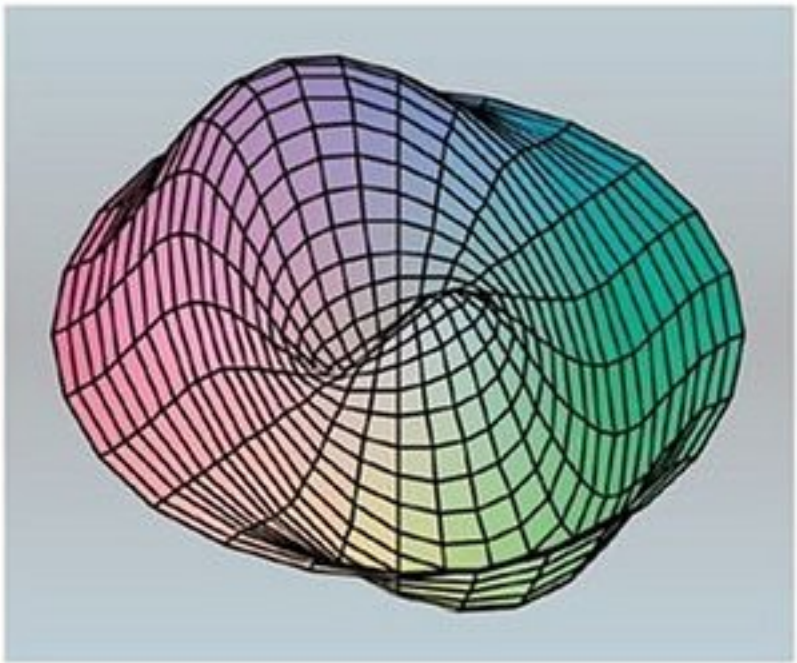
PHYSICS TEXTBOOK

WILEY-VCH

Frank Y. Wang

Physics with MAPLE

The Computer Algebra Resource for Mathematical Methods in Physics



Physics with Maple™

The Computer Algebra Resource for Mathematical Methods in Physics

Frank Y. Wang

WILEY-VCH Verlag GmbH & Co. KGaA

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Preface

Physics is guided by simple principles, but for many topics the physics tends to be obscured in the profusion of mathematics. As interactive software for computer algebra, Maple[†] can assist educators and students to overcome the obstacle of mathematical difficulties. The objective of this book is to introduce Maple both for teaching and learning physics by taking advantage of the mathematical power of symbolic computation, so that one can concentrate on applying the principles of *setting* equations, instead of technical details of *solving* equations.

Most physics textbooks were written before advanced computer software became conveniently available. The conventional approach to a topic places emphasis on theory and formalism, devoting many paragraphs to performing algebraic operations in deriving equations manually; other than some well known examples, most applications of theory are omitted. One reason that those examples are well known is that they admit analytic solution: they typically represent simplified situations that generally fail to fully reflect the reality. In most situations, analytic solutions simply do not exist, and one cannot proceed without the assistance of a computer. Although some books have sections discussing numerical methods, many of them contain just the theory of numerical methods, and one is required to possess programming skill for practice; this part is hence generally neglected. Essentially all experiments in physics measure numbers, so any formulation must eventually be reducible to numbers. Under a conventional curriculum, a student's ability to calculate and to extract numerical results from the formalism is somehow inadequate. The result is not surprising: a student may be weak in those areas, and he or she thus achieves only partial comprehension because of technical difficulties.

Maple can remedy some deficiency or weakness in traditional training. Using Maple, one can manipulate equations and diminish tedious paper work that distracts from the main focus of learning physics. It is particularly useful in problems that require extensive calculations, such as problems in calculus involving the chain rule, change of variables, and integration by parts. Maple is such a powerful software that an educator can introduce more advanced topics without being restricted to the presumed mathematical background of students, and a student can explore more advanced applications without fear of mathematical difficulty. From an analytic solution one can obtain numerical results by substituting numerical values. For equations that admit no analytic solution, one can, in practice, solve them numerically if proper initial conditions are supplied. An important feature of Maple is that it can produce

[†]Maple is a registered trademark of Maplesoft, a division of Waterloo Maple Inc.; see `http://www.maplesoft.com`.

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instant graphics to serve as a visual guide, which is generally the best way to understand the underlying physics.

Take the Bessel functions as an example: many students and even researchers find these so-called special functions alien, despite their frequent recurrence in diverse branches of physics. One reason is that the treatment of Bessel functions requires numerical methods, with which not everybody is adequately familiar. Many physicists have never produced a number from such functions, and a worked example of expansion in Bessel functions is lacking from most commonly used textbooks. Can we imagine a student learning the relations for the trigonometric functions and Fourier series without ever producing a number? Maple reduces routines of the Bessel functions to a simple command, which spares one from a tedious and protracted process of programming and debugging, and can produce plots interactively. The most effective way to learn such functions is to practise them, by calculating the expansion coefficients, similar to those in the Fourier series, and observing the graphical output. Maple can serve not only for pedagogical purposes: in practice it is much more convenient to evaluate coefficients for expansions in orthogonal functions with a computer than it is by long manual calculations.

There already exist many books on Maple, which indicates that Maple is a common but intrinsically complicated software. Maple contains literally thousands of commands and operators, from the most elementary to the quite complicated. Few people are proficient in every aspect of this software, not even the author! The purpose of this book is to use basic commands in Maple, so that one is not daunted by the software itself, to demonstrate what can be accomplished. From worked examples, a reader can develop a sense of knowing which problems are amenable to the assistance of Maple. This book is not intended for someone who seeks to explore diverse Maple commands; on the contrary, we generally limit ourselves to basic ones. Although Maple is a powerful software, it is not the only tool nor is it the perfect tool in mathematical physics. For some problems Maple can be of tremendous help, whereas for others an alternative approach might be more appropriate. Identifying the types of problem that are well suited to the capability of Maple is an important skill, and it is the main purpose of this volume.

This book is organized according to the fields of physics, covering classical mechanics, electromagnetism, relativity, quantum mechanics and statistical mechanics. We select problems that we consider suitable for Maple, and each is representative of its kind so that one can modify and adapt a worksheet for a similar problem. Our philosophy of solving problems is to apply Maple's capability to attack the mathematics in a direct fashion, so that we avoid digression into intricate mathematical manipulation. Because most problems admit no analytic solution, we particularly emphasize forming plots based on numerical solution. A graphic presentation of a solution provides the most enduring impression, and by experimenting through varying values of parameters and observing the graphic output, one can develop a sense of intuition and order of magnitude. A strong physical intuition toward a problem is arguably the most important asset of any physicist or engineer.

In our presentation, the relevant formulation precedes each problem; we devote particular attention to subjects that are less commonly presented in conventional textbooks but are crucial for computation. Mathematical formulas of the problem and results of calculations are out-

lined, omitting the details of intermediate steps. Our intention is to guide the reader with a clear mathematical objective through conventional equations and their symbols. The omitted portion of calculations is listed in the attached Maple worksheet, with a short explanation if it is not self-explanatory. In a worksheet, we attempt to perform most calculations using basic Maple commands. Other than using a "FOR" loop in some examples, we do not explicitly utilize the programming ability of Maple. In some situations, rearrangement and simplification of an expression are done manually; we avoid unnatural steps in Maple that might confuse readers. For most physical problems an alternative solution is practicable: we emphasize directness and consistency, not elegance.

Maple is interactive software, thus presenting worksheets in a static form constitutes a great challenge. Because the feature of this book is to use simple commands to solve physical problems, most Maple plots are generated in the default mode. Without optional commands to refine the plots, some of them might appear less satisfactory. Our compromise is based on our contention that commands purely for graph ornamentation are less important and potentially distracting for the purpose of this book. When one tries the worksheets on a computer, it is easy to discern the plots. In the same spirit, we believe that no matter how detailed the worksheet may be, the best way to learn Maple is to experiment with examples, and in this process one naturally learns the commands which are new or unfamiliar to one when first encountered in printed pages. Additionally, one should take advantage of the comprehensive index of Maple commands used in this book, which greatly facilitates learning by examples.

The first chapter is an illustration of basic algebraic operations with Maple, through their application to physics. Because most Maple commands are easy to understand, we hope that, even if one is unfamiliar with this software, one can follow those examples and develop a sense of the potential of Maple.

We begin our treatment of classical mechanics with oscillatory motion. Problems such as solving a system of equations and solving differential equations with constant coefficients, can be readily accomplished with Maple. We then introduce Lagrangian mechanics: this topic provides a perfect example for which Maple can be of great assistance. The required mathematics involves finding a function that extremizes an integral: this type of problem is called the calculus of variations, and calculations are typically extensive even for simple systems. We develop in Maple a method to derive the equation of motion without invoking an external library. We further use Maple's capability of solving differential equations, symbolically or numerically, to find the actual motion of a particle. With this method we can practically solve any problem in classical mechanics for which the Lagrangian function is known.

A chapter on expansion in orthogonal functions serves as a preparation for subsequent chapters. We start with the Fourier series; a task such as calculating the Fourier coefficients is a particularly valuable application of Maple. There is an even greater benefit in using Maple for expansions involving other orthogonal functions, most notably the Bessel functions: the latter topic is a common weakness among students. We present in detail many worked examples to demonstrate Maple's great utility for this purpose.

We then proceed to consider electromagnetism in static conditions. The fundamental concern of electromagnetism is to solve Maxwell's equations, and much of any course on this subject is devoted to vector calculus. To calculate an electric field and a magnetic field, we can perform integration directly from Coulomb's law and the Biot–Savart law. With Maple, we can concentrate on the physics, such as distinguishing the coordinates of the source point and the field point, and their separation, instead of properties of elliptic integrals. Maple provides the necessary operations such as gradient, curl and divergence in curvilinear coordinates, so that one has a minimal impediment of mathematics in learning the physics. We also introduce the theory of potential and harmonic functions, which is a direct application of expansion in orthogonal functions.

A chapter on circuits involves applications of solving a system of algebraic and differential equations, a topic similar to oscillatory motion. In that chapter we further use Maple's capability of complex numbers to treat problems of alternating-current circuits.

In our discussion of waves and optics, because a wave function contains both spatial and temporal components, Maple excels in producing animations that allow visualization. From simple motion and standing waves to advanced topics, such as a dispersion relation, which is important in quantum waves, animations illuminate both the spatial and temporal properties of waves. Physical optics involves the addition of waves: we approach this topic using Maple's graphic ability to display the final amplitude of waves in various combinations; Maple is certainly also capable of handling the summation of trigonometric functions.

Progressing to special relativity, while we recognize that the mathematics required in basic problems of special relativity is not particularly complicated, confusion arises from muddling between inertial frames. We avoid devious arguments, such as switching the frames of observers, and use Maple's capacity to solve equations so as to attack a problem directly.

After a short introduction to quantum phenomena, we present three chapters on quantum mechanics. This arguably most important topic comprises diverse elements of mathematical techniques. Most of the known solutions of prototypical problems are special functions, and Maple supports essentially all of them. In problems involving a piecewise-constant potential, one encounters transcendental equations; because a solution must be obtained from a graphical or numerical method, this topic is commonly ignored in conventional teaching. We offer several examples of this kind. We devote one chapter to quantum statistical mechanics, in which we extensively employ Maple to perform improper integrals exactly or approximately.

General relativity concludes the book. As stated above, physics is guided by simple principles: general relativity is the consummate example. Tremendously tedious calculations involving geometry in curved space contribute to a popular misconception that relativity is difficult. Maple allows one to perform these calculations so that one can focus on the elegance of physical ideas rather than being overwhelmed by mathematics. We deem this chapter particularly appropriate to end our book because it so clearly reflects our philosophy.

Niels Bohr felt that he never understood philosophical ideas until he had discussed them with himself in German, French and English, as well as in his native Danish. Because subtleties

typically arose during translation, he had to ponder the details so as to achieve a thorough mastery of the subject. Analogously, when we use Maple to solve a problem, we must translate the problem into a computer language. Unlike in a written or spoken language in which minor flaws might not impede communication, computer language requires accurate and precise input to produce the correct results. In this process we are compelled to examine the underlying physics in every layer. We believe that, through consideration of significant physical problems with computer software such as Maple, a student's understanding of physics is greatly strengthened.

Frank Y. Wang

New York City, August 2005

Guide for Users

The objective of this book is to enable a student to apply computer algebra to physical problems; most of these problems fall between intermediate and advanced undergraduate level, for a student who has completed general physics and calculus courses. By solving problems with Maple, one strengthens their physics knowledge, and acquires computer skills.

A trend in recent years for many physics textbooks is the inclusion of computer-related topics. For instance, the third edition of *Classical Electrodynamics* by Jackson, published in 1999, contains the following paragraph on page vii:

> Because of the increasing use of personal computers to supplement analytical work or to attack problems not amenable to analytic solution, I have included some new sections on the *principles* [Jackson's italics] of some numerical techniques for electrostatics and magnetostatics, as well as some elementary problems. ... The aim is to provide an understanding of such methods before blindly using canned software or even *Mathematica* or *Maple*.

There already exist numerous books on the *exposition* of the principles such as Jackson's; therefore, we focus on the *implementation* of the principles. Our book is intended for use in conjunction with standard traditional textbooks, see the Bibliography for a listing, on which we rely, but we avoid repeating their formal theoretical treatment. In the context of university physics education, we characterize our book as a supplement to introductory and intermediate courses, and a preparation for graduate studies.

From the point of view of both depth and breadth, we include more material in this book than an instructor can cover in one semester. To exploit the power of computer algebra, we select some difficult topics that are conventionally encountered in advanced courses. Never should a student feel discouraged – this book is packed with challenging problems and lengthy calculations. The exact analysis of real physical problems is usually complicated, (which constitutes the core of advanced courses), and because conventional teaching is restricted by the assumed mathematical background of students, most problems are set in an artificially idealized condition. With Maple one is empowered to pursue a more realistic situation beyond oversimplification. Even if a reader does not understand everything at once, it does not prevent them from experimenting with the worksheets to discover how they work, and in this process one begins building up the foundation for their advancement of knowledge in later years. The most important aspect for every topic is to discern the central physical ideas.

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Many exercises at the end of a chapter are sophisticated: they serve to provide additional information to the main text and to whet a student's appetite for advanced topics. One is not expected to be able to solve all of them, but nonetheless one should grasp the central ideas. Furthermore, identifying a problem for which solution with Maple is suitable is as important as solving that problem; for all chapters, an open-ended question is provided for the reader to discover problems from physics textbooks, and to create their own exercises by developing Maple worksheets to illustrate the advantage of an approach with computer algebra. Such an exercise provides research projects of infinite variety. The reader is strongly encouraged to export a Maple worksheet as `html` text, and to establish a website to display it or to submit it to the Maple Application Center at `www.mapleapps.com` for publication on the internet, so as to make it available to a wide audience.

Few textbooks are meant to be taught or read from cover to cover. To adopt this book for an integrated course, we classify chapters into five units. We recommend an instructor to follow Unit 1 first, then to select topics across other units according to students' backgrounds to tailor a suitable curriculum. Each unit also corresponds to an individual course typically offered in a physics department; it is practical for an instructor to adopt a unit as a supplement to a respective course.

Unit 1 **General Physics**

Chapter 1	Chapter 2	Chapter 9	Chapter 11	Chapter 13

This unit is suitable for students who have completed introductory physics courses: it delivers core skills such as solving equations, trigonometry, calculus, differential equations, complex numbers and computer graphics, through direct applications to physics. Chapter 1 alone serves as a comprehensive introduction to computation: the author has adopted it as one session in a required laboratory course and many students became instantly fascinated by the power of computer algebra and desired to explore this subject further.

Unit 2 **Classical Mechanics**

Chapter 3	Chapter 4

This unit is suitable for students who have completed, or are studying, classical mechanics at the level of Marion and Thornton.[1] We emphasize skills for the Lagrangian formulation of mechanics, which is indispensable for a student who intends to pursue advanced study in an area such as quantum field theory.

Unit 3 **Electromagnetism**

Chapter 5	Chapter 6	Chapter 7	Chapter 8	Chapter 10

[1] J. B. Marion and S. T. Thornton, *Classical Dynamics of Particles and Systems*, 4th ed., Fort Worth: Saunders College Publishing, 1995.

This unit is suitable for students who have completed, or are studying, electromagnetism at a level of Griffiths.[2] We utilize Maple's features on special functions and vector calculus for problems that require extensive calculations.

Unit 4 **Quantum Mechanics**

Chapter 14	Chapter 15	Chapter 16	Chapter 17

This unit is suitable for students who have completed, or are studying, quantum mechanics at the level of Gasiorowicz.[3] Employing Maple's great strength in differential equations, special functions and graphic ability, we systematically treat canonical problems based on wave mechanics. Chapter 17 on quantum statistics is applicable to a higher-level course on statistical mechanics, but prerequisites are minimal because the main difficulty of this topic is tedious mathematics for which Maple is particularly amenable.

Unit 5 **Relativity**

Chapter 12	Chapter 18

This unit is suitable for students who are interested in relativity, which typically occupies an elective course, although most students have exposure to special relativity in courses on electromagnetism, classical mechanics or modern physics. Chapter 18 on general relativity is the subject of numerous books at advanced level; our concise outline of the theory serves as a guide for the study of relevant literature, and our Maple worksheets provide concrete examples of actual calculations of tensor analysis that is generally presented abstractly.

* * * * *

A reasonably capable student should find this book a valuable companion throughout all the years of their undergraduate studies: it reinforces understanding of topics and courses previously encountered in only a traditional format, and enables one to employ computer algebra and associated powerful graphics to attack research problems.

Using a computer with a projector, the author has demonstrated the use of Maple during lectures in a classroom; we perform calculations using Maple, and defer or skip lengthy algebraic manipulation so that we maintain the focus of students on underlying physical principles. By introducing a topic with results generated almost instantly with Maple, we provide a preview of what a subsequent standard derivation on a blackboard eventually yields. For this purpose, graphic output allows an instructor to display a plot or an animation, which is far more efficient, accurate and illuminating than a manual sketch.

The Maple worksheets are available at

`http://faculty.lagcc.cuny.edu/fwang/maplebook` and

`http://www.wiley-vch.de/publish/en/books/ISBN3-527-40640-9/`,

and the author can be reached at `fw@phys.columbia.edu`.

[2] D. J. Griffiths, *Introduction to Electrodynamics*, 3rd ed., Upper Saddle River, NJ: Prentice Hall, 1999.

[3] S. Gasiorowicz, *Quantum Physics*, 3rd ed., New York: Wiley, 2003.

Bibliography

This book covers a broad range of topics. Our treatments are typically terse; they are intended to be representative, not comprehensive, and to complement the discussion of corresponding topics in traditional textbooks. Generally we omit derivation and simply state a theorem without proof. Our approach is to accept a theorem as true, and we focus on applications. For a reader who is interested in examining the details or exploring a topic further, the literature listed below should be beneficial. We limit our bibliography to a few books: they are either widely adopted textbooks or are available in the standard collection of a university library.

1. W. E. Boyce and R. C. Diprima, *Elementary Differential Equations and Boundary Value Problems*, 7th ed., New York: Wiley, 2001.

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1 Introduction

In this chapter we offer a brief introduction to Maple and its application to physics. We demonstrate Maple's capabilities in algebraic manipulations, graphs and calculus. Applying basic principles in mechanics to set equations, we employ Maple to solve physical problems; our approach is to learn Maple commands directly from working examples.

1.1 Overview

Maple is software for symbolic computation. With conventional software, calculations are restricted to numerical values, but Maple can manipulate symbolic expressions. For the most basic usage, Maple serves as a numeric calculator, as in the following examples. Using Maple to do numerical computations is straightforward: at the prompt sign >, one enters an expression, and terminates the input with a semicolon to have the result of a calculation displayed. A reader will best learn from this book by using his or her computer to try the examples; one should attempt to deduce the meaning of each command line before executing a calculation.

Worksheet 1.1

```
> 2*3 + 4/2;
```

$$8$$

```
> 2*(3+5)/4;
```

$$4$$

```
> 2^100;
```

$$1267650600228229401496703205376$$

```
> sqrt(179.0);
```

$$13.37908816$$

```
> 4/5 + 8/15;
```

$$\frac{4}{3}$$

```
> evalf(%);
```

$$1.333333333$$

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```
> sqrt(-4);
```
$$2\,I$$
```
> Pi;
```
$$\pi$$
```
> evalf(Pi, 20);
```
$$3.1415926535897932385$$
```
> exp(Pi);
```
$$e^{\pi}$$
```
> evalf(%);
```
$$23.14069264$$
```
> Pi^exp(1);
```
$$\pi^{(e)}$$
```
> evalf(%);
```
$$22.45915771$$

The first calculation obviously is to find 2 multiplied by 3, plus 4 divided by 2, and the result is 8; the precedence of arithmetical operations, such as multiplication before addition, follows convention, but parentheses can be applied as desired to impose another order of operations, such as the second example `2*(3+5)/4`. The third calculation contains a caret (`^`), which is Maple's notation for exponentiation, in this case to find 2 to the one hundredth power; the answer is displayed in 31 digits. To facilitate readability, spaces can be used liberally in an input command, but naturally not within a number or name.

Most Maple commands are self-explanatory. The command `sqrt(179.0)` serves to evaluate the square root of 179.0, which is 13.379. The most efficient way to learn a Maple command is to use the online help facility; to invoke help, one types a question mark followed by the name of the command.

`?`*command*

For instance, one can type `?sqrt` to discover additional information about this command. In most cases the help facility provides examples of usage. A rule of thumb is hence that, when one examines a worksheet that contains an unfamiliar command, one simply seeks help to elucidate the meaning.

An important feature of symbolic computation is shown in the calculation

$$\frac{4}{5}+\frac{8}{15}=\frac{4}{3};$$

Maple can perform it without converting fractions to decimals, and automatically simplifies the resulting fraction. A fraction is an exact quantity, and this calculation shows Maple's ability to perform exact computations. To obtain an approximate numerical result as a decimal number, we use the `evalf` command, which stands for "`evaluate` using `f`loating-point arith-

metic." The `evalf` command converts a fraction to its approximate value in decimal form. To learn more about this command, enter `?evalf`. The character `%` denotes the "ditto" operator, which recalls the previous result. The approximate value for $4/3$ is thus $1.333\ldots$.

Maple can handle complex numbers. In the example `sqrt(-4)`, Maple returns $2I$. The symbol `I` is a default character in Maple that denotes the square root of minus one, that is $I = \sqrt{-1}$.

Maple defines standard mathematical constants, such as π for the ratio of the circumference of a circle to its diameter, and e for the base of natural logarithms. Some characters and words are reserved in Maple because they have initially defined meanings for the system. For example, the letter `I` we have just seen to denote $\sqrt{-1}$, or `Pi` stands for π. We leave it as an exercise for readers to type `?Pi` to find more information about Maple's reserved words. Because Maple is case sensitive, we must ensure proper capitalization when calling these constants. As reserved words, such as `evalf` and `Pi`, have special meaning, we should refrain from using them for other purposes. Like any fraction, π is an exact quantity; to find its approximate value to a specified number of digits, such as 20 in the example shown, we employ the `evalf` command.

The exponential function e^x [or $\exp(x)$] is represented by the Maple function `exp(x)`. To invoke the number e, one should type `exp(1)`, or `exp(1.)` for its decimal approximation. We perform calculations to determine which value is greater – e^π or π^e, and the reader can answer this question from the Maple output.

Maple can do far more than basic numerical calculations. With further examples we demonstrate simple symbolic calculations and plotting capabilities.

Worksheet 1.2

```
> restart:
> g := (x+1)^3;
```

$$g := (x+1)^3$$

```
> g*(x+3);
```

$$(x+1)^3\,(x+3)$$

```
> expand(g);
```

$$x^3 + 3\,x^2 + 3\,x + 1$$

```
> expand(%%);
```

$$x^4 + 6\,x^3 + 12\,x^2 + 10\,x + 3$$

```
> Eq1 := a*x^2 + b*x + c = 0;
```

$$Eq1 := a\,x^2 + b\,x + c = 0$$

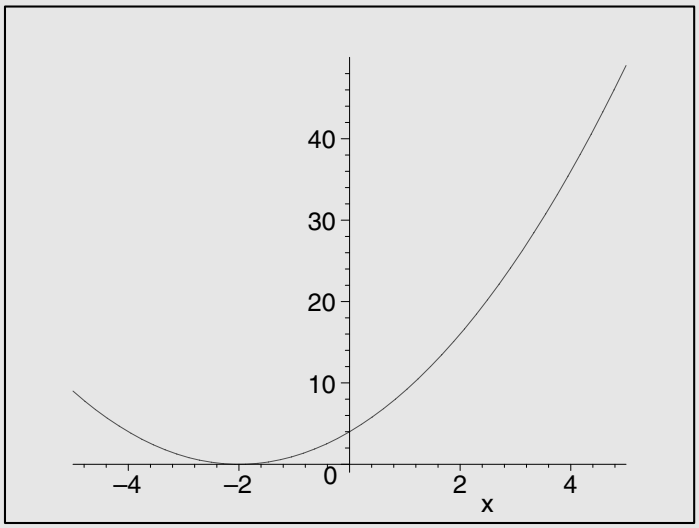
```
> Eq2 := solve({Eq1}, {x});
```

$$Eq2 := \left\{x = \frac{-b + \sqrt{b^2 - 4\,a\,c}}{2\,a}\right\}, \left\{x = \frac{-b - \sqrt{b^2 - 4\,a\,c}}{2\,a}\right\}$$

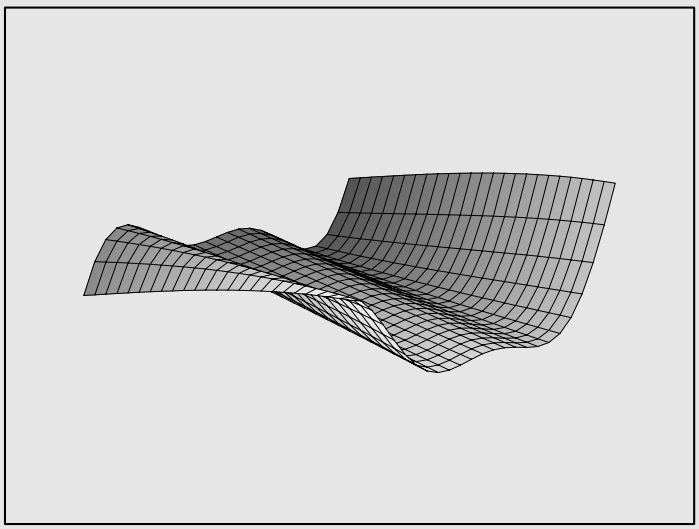
```
> solve({a1*x + b1*y = c1, a2*x + b2*y = c2}, {x, y});
```

$$\left\{x = \frac{b2\ c1 - c2\ b1}{-a2\ b1 + a1\ b2}, y = \frac{-a2\ c1 + a1\ c2}{-a2\ b1 + a1\ b2}\right\}$$

```
> plot(x^2 + 4*x + 4, x=-5..5);
```




```
> plot3d(x^2*sin(x-y), x=-Pi..Pi, y=0..1);
```



In this worksheet, we begin with a command `restart`, which clears previous assignments from the computer memory. In succeeding worksheets, we omit listing this command `restart`, but it is important to execute this to avoid interference from preceding calculations in the same session.

To assign a Maple expression to a name, one uses this syntax.

name `:=` *expression*`;`

In the example `g := (x+1)^3;`, we assign the expression $(x+1)^3$ to a symbol `g` that becomes the name to represent that expression. We can then manipulate the expression $(x+1)^3$ with a shorthand notation `g`, such as multiplying by another expression, or expansion using the command `expand`. To recall the previous result but one, we employ a double ditto operator `%%`; in this example we expand the expression $(x+1)^3(x+3)$ symbolically.

We can also specify a name for an equation: in an example we assign the general form of a quadratic equation to `Eq1`. We next introduce one of Maple's most important commands `solve`. This command is a general-purpose equation solver; it takes a single equation or a system of equations and attempts to solve exactly for a specified unknown or unknowns. To solve a single equation for a single unknown, the syntax is shown in the worksheet. To solve a system of equations, we provide equations in a set separated by commas within braces `{...}`, and instruct to solve for unknowns in a set also specified within braces.

Graphical presentation of a mathematical function generally provides the most illuminating way to understand properties of that function. To plot an explicit function of a single variable, one specifies the expression and the corresponding domain to the `plot` command. In the example above, we plot the equation $y = x^2 + 4x + 4$, with a domain of x from -5 to $+5$. This two-dimensional plot is the most elementary form. For more elaborate effects, such as line style, title, legend, and so forth, one can find information by invoking `?plot[options]`. We can plot a function of two variables as a surface in three-dimensional space, with the `plot3d` command for an expression f of x and y. In our example, we plot the equation $z = x^2 \sin(x - y)$, for x from $-\pi$ to π, and for y from 0 to 1.

Solving problems in calculus is a practical application of Maple. We offer the following worksheet to demonstrate Maple's capability in this subject.

Worksheet 1.3

```
> y := sin(4*x)*cos(x);
```

$$y := \sin(4\,x)\cos(x)$$

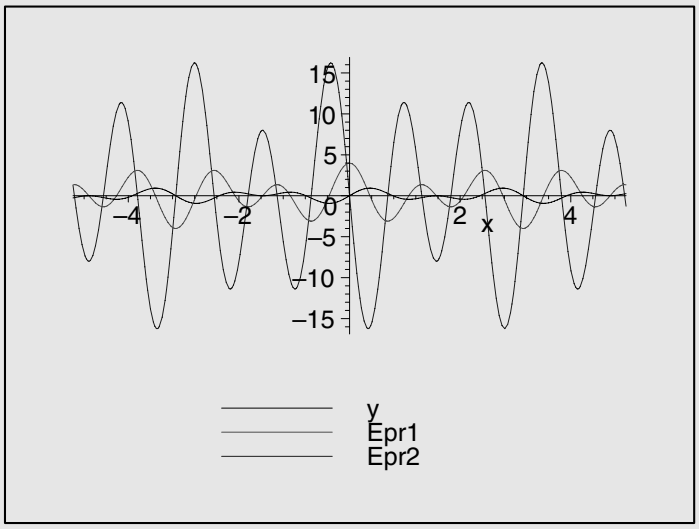
```
> Epr1 := diff(y, x);
```

$$Epr1 := 4\cos(4\,x)\cos(x) - \sin(4\,x)\sin(x)$$

```
> Epr2 := diff(y, x$2);
```

$$Epr2 := -17\sin(4\,x)\cos(x) - 8\cos(4\,x)\sin(x)$$

```
> plot([y, Epr1, Epr2], x=-5..5, legend=["y", "Epr1", "Epr2"]);
```




```
> int(a + b*x + c*x^2, x);
```

$$a\,x + \frac{b\,x^2}{2} + \frac{c\,x^3}{3}$$

```
> int(csc(x), x);
```

$$-\ln(\csc(x) + \cot(x))$$

```
> Int(1/(a^2+x^2), x);
```

$$\int \frac{1}{a^2 + x^2}\,dx$$

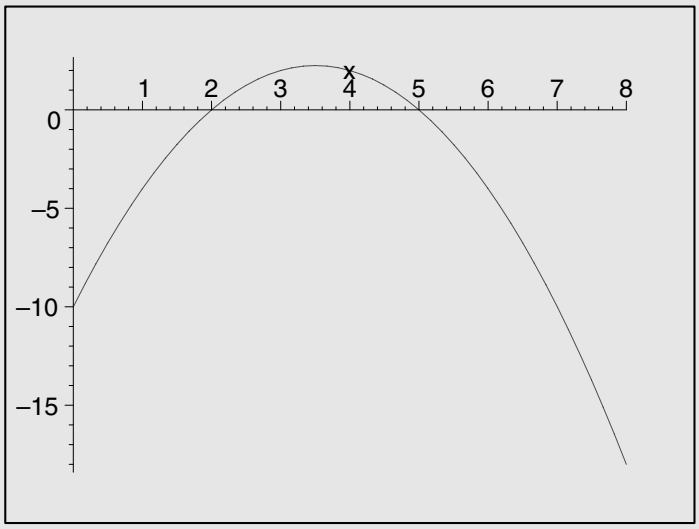
```
> value(%);
```

$$\frac{\arctan\left(\frac{x}{a}\right)}{a}$$

```
> Epr3 := -x^2 + 7*x - 10;
```

$$Epr3 := -x^2 + 7\,x - 10$$

```
> plot(Epr3, x=0..8);
```




```
> int(Epr3, x=2..5);
```

$$\frac{9}{2}$$

```
> Eq4 := diff(u(t),t$2) + 5*diff(u(t),t) + 6*u(t) = 0;
```

$$Eq4 := \left(\frac{d^2}{dt^2}\,\mathrm{u}(t)\right) + 5\,\left(\frac{d}{dt}\,\mathrm{u}(t)\right) + 6\,\mathrm{u}(t) = 0$$

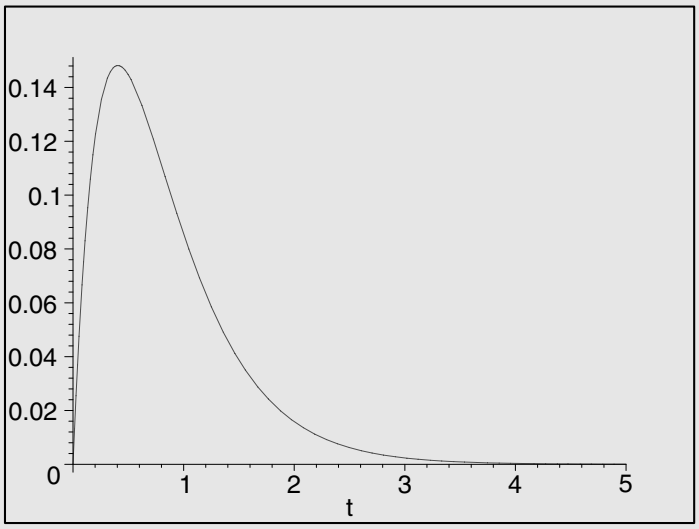
```
> dsolve({Eq4, u(0)=0, D(u)(0)=1}, {u(t)});
```

$$\mathrm{u}(t) = -e^{(-3\,t)} + e^{(-2\,t)}$$

```
> soln := rhs(%);
```

$$soln := -e^{(-3\,t)} + e^{(-2\,t)}$$

```
> plot(soln, t=0..5);
```



The commands for differentiation and integration are readily recognizable from the above examples. The syntax to find $\frac{d}{dx}f(x)$ is `diff(f(x), x)`. A sequence operator `$` is useful for higher-order derivatives; for example, to find the second derivative of $f(x)$, we write `diff(f(x), x$2)`. We first assign the expression $\sin(4x)\cos(x)$ to a name `y`, then find its first and second derivatives with Maple's `diff` command. We obtain

$$\frac{d}{dx}\sin(4x)\cos(x) = 4\cos(4x)\cos(x) - \sin(4x)\sin(x),$$

$$\frac{d^2}{dx^2}\sin(4x)\cos(x) = -17\sin(4x)\cos(x) - 8\cos(4x)\sin(x).$$

When we specify multiple functions separated by commas within square brackets to `plot`, we present them in the same plot. Maple provides several structures for collections of items, including sequence, list and set. Items in a sequence are simply separated with commas. Such a sequence enclosed within square brackets `[...]` becomes a *list*, and enclosure of a sequence within braces `{...}` prepares a *set*. In some situations a list and a set are actually interchangeable, but a distinction between these structures is that order and repetition are preserved in a list but not in a set. For the `solve` command in a preceding worksheet, the order of equations does not affect the solution; thus we use a set. For the `plot` command in this worksheet, we intend to specify a legend for each curve, for which order is important; thus we use a list.

The syntax to evaluate an indefinite integral $\int f(x)dx$ is `int(f(x), x)`. For two formulas according to above examples, we find that

$$\int (a + bx + cx^2)\,dx = ax + \frac{1}{2}bx^2 + \frac{1}{3}cx^3,$$

and

$$\int \csc(x)\,dx = -\ln[\csc(x) + \cot(x)].$$

If we capitalize `I` in `Int`, Maple returns the integral unevaluated but in a "prettyprinted" format; we can use the `value` command to evaluate the integral. Using `Int` and `value` in a pair is very useful in catching typographical errors such as misplaced parentheses. Although we do not use `Int` in the rest of the book because of limitations of space, the reader can easily modify the worksheet to see what is typed. Definite integration can also be performed; for example,

$$\int_2^5 (-x^2 + 7x - 10)\,dx = \frac{9}{2}.$$

In the Maple instruction the upper and lower limits are specified in the form of a range on the integration variable. This result appears as a fraction, which illustrates again that by default Maple performs an exact calculation, hence without approximation.

Maple can solve differential equations, with the `dsolve` command. For this differential equation,

$$\frac{d^2}{dt^2}u(t) + 5\frac{d}{dt}u(t) + 6u(t) = 0,$$

we specify these initial conditions:

$$u(0) = 0, \quad \left.\frac{du(t)}{dt}\right|_{t=0} = 1.$$

The usage of the `dsolve` command is indicated in the worksheet; in a similar way to the format with `solve`, we provide a differential equation and initial conditions as a set. In the differential equation, we must enter the unknown function as `u(t)` to specify that `u` is a function of `t`. In initial conditions, we can use the differential operator `D`. The meaning of the argument is `D(f)(x)=diff(f(x), x)`. The expression `D(f)(0)` thus defines the first derivative of f evaluated at 0. Maple solves this differential equation directly and gives a solution

$$u(t) = -e^{-3t} + e^{-2t}.$$

From the Maple output, we extract the right side of the solution with the `rhs` command, and plot this expression.

Through these worksheets, we acquire a taste of Maple, and we learn a few Maple commands. With these commands we can manipulate and plot algebraic expressions, solve equations, perform operations of differential and integral calculus, and solve differential equations. Effective usage of these basic commands can greatly improve our productivity. In the rest of this chapter, we employ Maple to solve physical problems in illustrating the application of Maple to physics. We introduce further commands when we encounter a situation that warrants it, to provide a reader with the context of its utility.

1.2 Basic Algebra and Solving Equations

We mentioned that Maple's `solve` command is exceedingly useful. In this section we apply it directly to solve real physical problems.

Example 1.1 From elementary mechanics, the necessary conditions for static equilibrium of an object are that vector sums of the forces and the torques about any axis are zero:

$$\sum \mathbf{F} = 0, \tag{1.1}$$

$$\sum \mathbf{N} = 0. \tag{1.2}$$

This type of problem involves solving several equations simultaneously; such a task can be tedious as manual work, but it can be readily accomplished with Maple.

Consider a problem from an introductory physics textbook: a stepladder of negligible weight is constructed as shown in Figure 1.1.[1] A man of mass 70.0 kg stands on the ladder 3.0 m from the bottom in a direction parallel to the leg of the ladder. Assuming the floor to be frictionless, we seek to evaluate the tension in the horizontal bar, the normal force for each leg, and the components of the reaction force at the single hinge at the top.

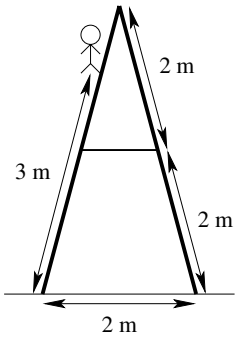


Figure 1.1: A man on a ladder.

Solution It is convenient to treat each half of the ladder separately. The free-body diagram appears in Figure 1.2. The man of mass 70.0 kg exerts a force $mg = (70.0 \text{ kg})(9.8 \text{ m s}^{-2}) = 686.0$ N. The angle θ, defined in the following diagram, is calculated from geometry,

$$\cos\theta = \frac{1.0}{4.0}.$$

From the left half of the ladder, equilibrium of forces of the x component gives

$$\sum F_x = 0, \quad T - R_x = 0,$$

[1] This problem is similar to one in Halliday, Resnick and Walker 2005, p. 731, problem 77.

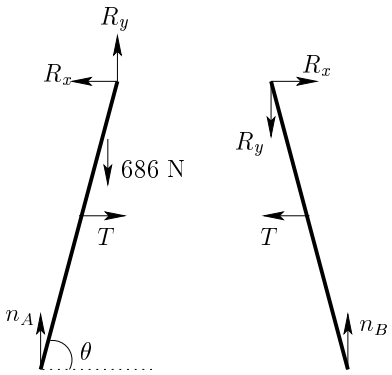


Figure 1.2: Free-body diagram.

and for the y component,

$$\sum F_y = 0, \quad R_y + n_A - 686 = 0.$$

Choosing the top of the ladder as the pivot, we find for equilibrium of torques

$$\sum N_l = 0, \quad (686)(1.0)(\cos\theta) + (T)(2.0)(\sin\theta) - (n_A)(4.0)(\cos\theta) = 0.$$

From the right half, equilibrium of forces in the y component gives

$$\sum F_y = 0, \quad n_B - R_y = 0,$$

and equilibrium of torques gives

$$\sum N_r = 0, \quad (n_B)(4.0)(\cos\theta) - (T)(2.0)(\sin\theta) = 0.$$

Because we have five equations, and five unknowns – n_A, n_B, R_x, R_y and T, we can solve these five equations simultaneously.

Worksheet 1.4 We first perform a simple calculation: $(70.0)(9.8) = 686.0$. To evaluate θ, we use the `arccos` command. Entering five equations above, we assign them as `Eq1`, `Eq2`, ..., `Eq5`. We insert these five equations as a set (separated by commas and enclosed within braces) to `solve`, and evaluate the five unknowns.

```
> m := 70; g := 9.8;
```

$$m := 70$$
$$g := 9.8$$

```
> m*g;
```

$$686.0$$

```
> theta := arccos(1.0/4.0);
```

$$\theta := 1.318116072$$

```
> Eq1 := Rx - T = 0;
```

$$Eq1 := Rx - T = 0$$

```
> Eq2 := nA + Ry - 686.0 = 0;
```

$$Eq2 := nA + Ry - 686.0 = 0$$

```
> Eq3 := 686.0*1.0*cos(theta) + T*2.0*sin(theta) -
> nA*4.0*cos(theta);
```

$$Eq3 := 171.4999998 + 1.936491673\,T - 0.9999999988\,nA$$

```
> Eq4 := nB - Ry = 0;
```

$$Eq4 := nB - Ry = 0$$

```
> Eq5 := nB*4.0*cos(theta) - T*2.0*sin(theta) = 0;
```

$$Eq5 := 0.9999999988\,nB - 1.936491673\,T = 0$$

```
> solve({Eq1, Eq2, Eq3, Eq4, Eq5}, {nA, nB, Rx, Ry, T});
```

$$\{T = 132.8433286,\ nB = 257.2500000,\ nA = 428.7500000,\ Ry = 257.2500000,\ Rx = 132.8433286\}$$

We find that the tension is

$$T = 132.8\,\text{N},$$

the normal forces for each leg are

$$n_A = 428.8\,\text{N}, \quad n_B = 257.3\,\text{N},$$

and the x and y components of the reaction force at the hinge are

$$R_x = 132.8\,\text{N}, \quad R_y = 257.2\,\text{N}.$$

Example 1.2 For a collision of two particles, we assume the net external force on this system to be zero. Under this condition, the linear momentum is conserved,

$$\mathbf{F} = \frac{d\mathbf{p}}{dt} = 0, \quad \mathbf{p} = \text{constant}. \tag{1.3}$$

For an elastic collision the kinetic energy is also conserved. These conserved quantities enable us to calculate the velocities of the two particles after collision.

Consider the elastic collision in one dimension shown in Figure 1.3: particle 1 with mass m_1 moves with initial velocity v_{1i}, and particle 2 with mass m_2 moves with initial velocity v_{2i}. Because $v_{1i} > v_{2i}$, particle 1 will catch up with particle 2. Find the final velocities of particles 1 and 2 after the collision.

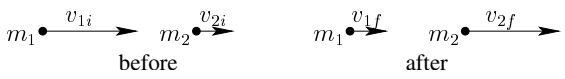


Figure 1.3: One-dimensional collision problem.

Solution We know that both momentum and kinetic energy are conserved, which yield these two equations:

$$m_1 v_{1i} + m_2 v_{2i} = m_1 v_{1f} + m_2 v_{2f}, \tag{1.4}$$

and

$$\frac{1}{2} m_1 v_{1i}^2 + \frac{1}{2} m_2 v_{2i}^2 = \frac{1}{2} m_1 v_{1f}^2 + \frac{1}{2} m_2 v_{2f}^2. \tag{1.5}$$

Solving these two equations simultaneously, we can find v_{1f} and v_{2f}. Because undertaking this calculation manually is tedious, we use Maple's `solve` command to accomplish this task.

Worksheet 1.5 It is straightforward to enter these two equations and to use the `solve` command.

```
> Eq1 := m1*v1i + m2*v2i = m1*v1f + m2*v2f;
```

$$Eq1 := m1\ v1i + m2\ v2i = m1\ v1f + m2\ v2f$$

```
> Eq2 := 1/2*m1*v1i^2 + 1/2*m2*v2i^2 = 1/2*m1*v1f^2 + 1/2*m2*v2f^2;
```

$$Eq2 := \frac{m1\ v1i^2}{2} + \frac{m2\ v2i^2}{2} = \frac{m1\ v1f^2}{2} + \frac{m2\ v2f^2}{2}$$

```
> solve({Eq1, Eq2}, {v1f, v2f});
```

$$\{v1f = v1i,\ v2f = v2i\},$$
$$\left\{v2f = \frac{m2\ v2i - v2i\ m1 + 2\,m1\ v1i}{m2 + m1},\ v1f = \frac{-v1i\ m2 + m1\ v1i + 2\,m2\ v2i}{m2 + m1}\right\}$$

As the second equation is quadratic in velocities, Maple returns two sets of solutions; we select the non trivial one,

$$v_{1f} = \frac{m_1 v_{1i} - m_2 v_{1i} + 2 m_2 v_{2i}}{m_1 + m_2}, \quad v_{2f} = \frac{m_2 v_{2i} - m_1 v_{2i} + 2 m_1 v_{1i}}{m_1 + m_2}. \tag{1.6}$$

We employ two examples in this section to demonstrate the usage of the `solve` command. After application of physical principles, solution of this type of problems requires essentially no skill other than basic algebra, but manually performing repetitive substitutions, cancellations and simplifications can be laborious; they represent examples for which Maple proves useful and convenient. If one does not consider such a problem of an elastic collision tedious, try a

problem in Section 12.2, in which we solve a problem of collision that takes into account the relativistic effect. The basic idea is simple: the mass of a body increases with velocity; thus we must modify the mass by a factor of $(1 - v^2/c^2)^{-1/2}$. The presence of square roots makes solving the equations awkward; calculations typically extend over many pages of paper. With Maple, we simply apply the principle of relativity to set the equations, and the rest is left to Maple to solve the equations!

1.3 Calculus

Performing calculations involving operations of differential and integral calculus constitutes a major task in solving physical problems. One can in principle differentiate any continuous function, employing techniques such as the chain rule; many calculations are merely repetitive. For example, one can try to calculate this second derivative:

$$\frac{d^2}{dx^2}\sin(4x)\cos(x).$$

The calculation is straightforward to undertake: one only needs to be patient and careful to perform it term by term. In contrast, we have demonstrated that Maple can perform it quickly and reliably. This facility is particularly useful in expanding a function as a Taylor series, which we will discuss in Section 2.1.

Integration is a much more complicated process than differentiation. Some applicable techniques are change of variables and integration by parts, but for other than basic functions there is no general rule for performing an integration. For example, evaluating the integral $\int \csc(x)\,dx$ is not so obvious. Essentially, because an indefinite integral corresponds to an antiderivative, for an integral

$$g(x) = \int f(x)\,dx, \tag{1.7}$$

we seek a function $g(x)$ such that

$$\frac{d}{dx}g(x) = f(x). \tag{1.8}$$

We can search an integral table in a mathematical handbook for this purpose. No matter how extensive a table might be, one typically needs to make a suitable substitution so that an integrand conforms to that listed in the table, which can itself be a tedious task. Employing Maple to perform an indefinite integration we can regard as an implicit "computer search" to expedite the process, with most required transformations also automatically undertaken.

A definite integral

$$\int_{x_1}^{x_2} f(x)\,dx \tag{1.9}$$

is defined as the area bounded between a curve defined by $f(x)$ and the x axis, between two specified values x_1 and x_2. In principle, such an area can be calculated as

$$\lim_{\Delta x_i \to 0} \sum_i f(x_i)\Delta x_i. \tag{1.10}$$

In practice, it is possible to conduct definite integration numerically by letting Δx_i become small and adding all $f(x_i)\Delta x_i$ in a designated range. It is reasonable to expect Maple to perform numerical integration also.

We choose three integrals to test Maple's capability and to illustrate its utility.

Example 1.3 Evaluate the following integrals:

1.
$$\int_0^\infty \left[x^2\left(\frac{1}{2x^2} + x\sqrt{x^2+2} - 1 - x^2\right)\right] dx; \tag{1.11}$$

2.
$$\int_0^1 \frac{1}{\sqrt{1-\Omega+x^{-2}\Omega}}\, dx; \tag{1.12}$$

3.
$$\int_0^1 \frac{1}{\sqrt{1-\Omega+x^{-1}\Omega}}\, dx, \quad \text{for } \Omega > 1. \tag{1.13}$$

As a justification for such calculations, the first integral appears in evaluating the energy of a system that consists of mutually interacting particles, a subject of advanced quantum statistical mechanics. The second and third integrals are involved in calculating the age of the universe according to specific models.[2] We will discuss statistical mechanics in Chapter 17, and cosmology in Chapter 18.

Solution Although no integrand appears complicated, performing these integrations is intricate. One can consult an integral table for a particular standard form. For instance, one can find

$$\int x^3\sqrt{x^2+a^2}\, dx = \left(\frac{x^2}{5} - \frac{2a^2}{15}\right)\sqrt{(a^2+x^2)^3}, \tag{1.14}$$

which is useful for the first integral, but naturally we can invoke Maple to spare us this trouble.

Worksheet 1.6 We simply type the integrand and use the `int` command to evaluate the integrals. Infinity ∞ is entered as `infinity`. We introduce the `assuming` command to inform Maple about conditions imposed in performing calculations within that integration.

[2] E. W. Kolb and M. S. Turner, *The Early Universe*, Redwood City, CA: Addison-Wesley, 1990, p. 52.

```
> Epr1 := x^2*(1/(2*x^2) + x*sqrt(x^2 + 2) - 1 - x^2);
```

$$Epr1 := x^2 \left(\frac{1}{2\,x^2} + x\sqrt{x^2+2} - 1 - x^2 \right)$$

```
> Epr2 := int(Epr1, x);
```

$$Epr2 := \frac{x^2\,(x^2+2)^{(3/2)}}{5} - \frac{4\,(x^2+2)^{(3/2)}}{15} + \frac{x}{2} - \frac{x^3}{3} - \frac{x^5}{5}$$

```
> Epr3 := int(Epr1, x=0..infinity);
```

$$Epr3 := \frac{8\sqrt{2}}{15}$$

```
> Epr4 := int(1/sqrt(1 - Omega + Omega/x^2), x=0..1);
```

$$Epr4 := \frac{\sqrt{\Omega} - 1}{-1 + \Omega}$$

```
> Epr5 := int(1/sqrt(1 - Omega + Omega/x), x=0..1) assuming
Omega>1;
```

$$Epr5 := \frac{1}{4} \frac{-\Omega\pi + \Omega^2\pi - 4(-1+\Omega)^{(3/2)} - 2\Omega \arcsin\left(\frac{-2+\Omega}{\Omega}\right) + 2\Omega^2 \arcsin\left(\frac{-2+\Omega}{\Omega}\right)}{(-1+\Omega)^{(5/2)}}$$

For the first integral in indefinite form, Maple yields a result

$$\int \left[x^2 \left(\frac{1}{2x^2} + x\sqrt{x^2+2} - 1 - x^2 \right) \right] dx = \frac{x}{2} + \frac{x^2(x^2+2)^{3/2}}{5} - \frac{4(x^2+2)^{3/2}}{15} - \frac{x^3}{3} - \frac{x^5}{5},$$

which is consistent with what we find in a table. This problem concerns an improper integral, which involves an end point at infinity. It seems that this improper integral diverges, because each term produces an infinite number. Using Maple to make the calculation, we obtain

$$\int_0^\infty \left[x^2 \left(\frac{1}{2x^2} + x\sqrt{x^2+2} - 1 - x^2 \right) \right] dx = \frac{8\sqrt{2}}{15}, \tag{1.15}$$

which is finite and exact! The reason is that, as one infinity cancels another, we obtain a net result that is a finite number. In treatments of numerous mutually interacting particles, infinity typically appears in calculations, which constitutes a major mathematical challenge. Many great physicists considered ways to cancel one infinity with another so as to obtain a finite result. The above calculation was a celebrated achievement in statistical mechanics published in *Physical Review* in 1957 by two Nobel laureates.[3]

For the second and third integrals, we refrain from repeating results from the Maple output, but merely indicate to the reader that a simple integrand can yield a complicated result. It

[3] T. D. Lee and C. N. Yang, "Many-body problem in quantum mechanics and quantum statistical mechanics," *Physical Review*, **105**, 1119–1120 (1957).

is possible that your version of Maple cannot execute these integrals (or display the results differently), which would exemplify the fact that Maple is not omnipotent. We need not be concerned with these integrals for now. Maple is capable of producing undesired results, and we take this opportunity to remind the reader that it is often necessary to manually check the results obtained by Maple. In many calculations of integrals, signs of parameters are important. For example, to proceed to calculate the third integral, we must know the sign of $1-\Omega$; for this reason we provide Maple with such information using the `assuming` command. The latter command has only a local effect; if one seeks to impose an assumption on a specified variable or name for the entire worksheet, one should use the `assume` command, of which we present an example shortly.

1.4 Differential Equations

An equation containing derivatives of an unknown function is called a differential equation. Many a problem in physics is formulated as a differential equation. For example, the most famous, Newton's second law,

$$F = ma, \tag{1.16}$$

is expressed explicitly as this differential equation:

$$F\left(t, x(t), \frac{d}{dt}x(t)\right) = m\frac{d^2}{dt^2}x(t). \tag{1.17}$$

Differential equations are closely related to integration: indeed, by definition, evaluating the integral

$$g(x) = \int f(x)\,dx$$

is equivalent to solving the differential equation

$$\frac{d}{dx}g(x) = f(x).$$

Finding solutions of differential equations is an even greater challenge than integration. There exist techniques such as separation of variables and integrating factor, but there is no single direct approach that one can universally apply to a differential equation. The essential objective in solving a differential equation is to find a function that satisfies the differential equation. Adopting the same point of view as for integration, we regard that we invoke Maple as an assistance to find such a function.

One can easily write a differential equation that Maple cannot solve exactly, which generally implies that such a differential equation admits no analytic solution. In fact, one must be extremely lucky to have a differential equation that both reflects the reality of an experimental

situation and admits an exact solution. For most equations numerical methods are inevitable. The concept of numerical solution of a differential equation is similar to that of numerical integration, which we will discuss in Chapter 2. In practice, there are many effective numerical algorithms, many of them having been coded as routines in computer languages such as C or FORTRAN. Maple has implemented most numerical methods so that they become readily available to a user in a simple line command. This facility enables great flexibility and convenience in investigating a differential equation without a tedious and protracted process of programming and debugging. Combining `dsolve` with the plot facility, we can visualize the result immediately. In this book we strongly emphasize forming plots based on numerical solutions.

1.4.1 Exact Solutions

Example 1.4 A sky diver of mass m falls vertically downward. At time $t = 0$, she attains a velocity v_0, and opens the parachute. The force of air resistance is proportional to the velocity. Find the velocity of the sky diver after time $t = 0$.

Solution Assuming the force of air resistance to be

$$F_d = bv(t),$$

and using Newton's second law, we set a differential equation

$$mg - bv(t) = m\frac{d}{dt}v(t). \tag{1.18}$$

For this simple first-order differential equation, one can readily find a general solution in any textbook on differential equations:

$$v(t) = \frac{mg}{b} + c_1 e^{-bt/m}. \tag{1.19}$$

This general solution contains an undetermined coefficient c_1, arising as a constant of integration. Although Maple invariably omits the constant of integration in the result of an indefinite integral, the solution of a differential equation is output with the correct integration constants. To choose a particular value that is consistent with our physical situation in this case, we must identify a particular point, commonly the initial velocity $v(t = 0) = v_0$. With this condition, we have

$$v(t = 0) = \frac{mg}{b} + c_1 = v_0, \quad c_1 = v_0 - \frac{mg}{b}.$$

The solution of the given initial-value problem is therefore

$$v = \frac{mg}{b} + \left(v_0 - \frac{mg}{b}\right) e^{-bt/m}. \tag{1.20}$$

Maple can solve an initial-value problem; it can also find the general solution. In the following worksheet we introduce some techniques of algebraic manipulation using the `eval` and `subs` commands.

Worksheet 1.7 We employ the `dsolve` command to solve equation (1.18), and obtain a general solution that contains an undetermined coefficient, $_C1$. The `eval` command serves to evaluate the solution at $t = 0$. After we find $_C1$ using `solve`, we can substitute it into the general solution, also using `eval` or with the `subs` command. We can avoid all these operations by simply providing Maple with an initial condition in `dsolve` as shown in `Eq6`.

```
> Eq1 := m*diff(v(t), t) = m*g - b*v(t);
```

$$Eq1 := m\,(\tfrac{d}{dt}\,\mathrm{v}(t)) = m\,g - b\,\mathrm{v}(t)$$

```
> Eq2 := dsolve(Eq1, v(t));
```

$$Eq2 := \mathrm{v}(t) = \frac{g\,m}{b} + e^{(-\frac{b\,t}{m})}\,_C1$$

```
> Eq3 := v0 = eval(rhs(Eq2), t=0);
```

$$Eq3 := v0 = \frac{g\,m}{b} + _C1$$

```
> Eq4 := solve({Eq3}, {_C1});
```

$$Eq4 := \left\{_C1 = \frac{v0\,b - m\,g}{b}\right\}$$

```
> Eq5 := subs(Eq4, Eq2);
```

$$Eq5 := \mathrm{v}(t) = \frac{g\,m}{b} + \frac{e^{(-\frac{b\,t}{m})}\,(v0\,b - m\,g)}{b}$$

```
> Eq6 := dsolve({Eq1, v(0)=v0}, v(t));
```

$$Eq6 := \mathrm{v}(t) = \frac{g\,m}{b} + \frac{e^{(-\frac{b\,t}{m})}\,(v0\,b - m\,g)}{b}$$

1.4.2 Special Functions

Certain types of differential equation appear repeatedly in diverse branches of physics. Many of them are profoundly investigated and have well established solutions, to which one refers as special functions. For example, Bessel's equation,

$$x^2\frac{d^2}{dx^2}y(x) + x\frac{d}{dx}y(x) + (x^2 - \nu^2)y(x) = 0, \tag{1.21}$$

appears in boundary-value problems in electrostatics, in the wave equation, in optics, in the Schrödinger equation – to name only a few. Solutions of this differential equation are called Bessel functions.

We employ Maple to solve this equation directly.

Worksheet 1.8

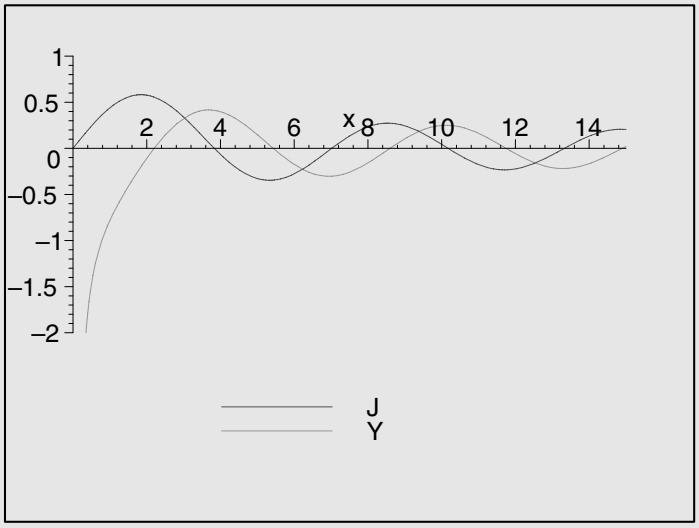
```
> Eq1 := x^2*diff(y(x),x$2) + x*diff(y(x),x) + (x^2 - nu^2)*y(x)
> = 0;
```

$$Eq1 := x^2 \left(\frac{d^2}{dx^2}\,\mathrm{y}(x)\right) + x \left(\frac{d}{dx}\,\mathrm{y}(x)\right) + (x^2 - \nu^2)\,\mathrm{y}(x) = 0$$

```
> Eq2 := dsolve(Eq1, y(x));
```

$$Eq2 := \mathrm{y}(x) = _C1\ \mathrm{BesselJ}(\nu,\, x) + _C2\ \mathrm{BesselY}(\nu,\, x)$$

```
> plot([BesselJ(1,x), BesselY(1,x)], x=0..15, -2..1, legend=["J",
> "Y"]);
```



In the Maple output, we discern `BesselJ` and `BesselY`, which are Bessel functions. Because the Bessel equation is a second-order differential equation, we have two independent solutions with two undetermined coefficients $_C1$ and $_C2$, which can be found from imposed boundary conditions. We plot the Bessel functions; from the graph, we see that `BesselY` diverges at $x = 0$: if the domain of our interest includes $x = 0$, we must therefore reject `BesselY`. We can also observe visually the locations of roots of Bessel functions, at which the curve crosses the x axis, which are important in many calculations. This example demonstrates the utility of a graphical representation of a function. For an eager reader, the `fsolve` command can be used to locate the roots; see Section 5.5.

1.4.3 Numerical Solutions

A fact that we must bear in mind is that, for most physical systems, analytic solutions simply do not exist. Problems appearing in most textbooks that admit exact solutions in closed form generally reflect an idealized situation. We take the following simple problem as an example.

Example 1.5 One can make an experimental arrangement shown in Figure 1.4: a cart of mass m_1 is released at rest from $x = 0$ at $t = 0$, and is dragged along a table by another mass m_2 descending from an elevated position. Assuming both the surface of the table and the pulley to be frictionless, find the position of m_1 as a function of time.

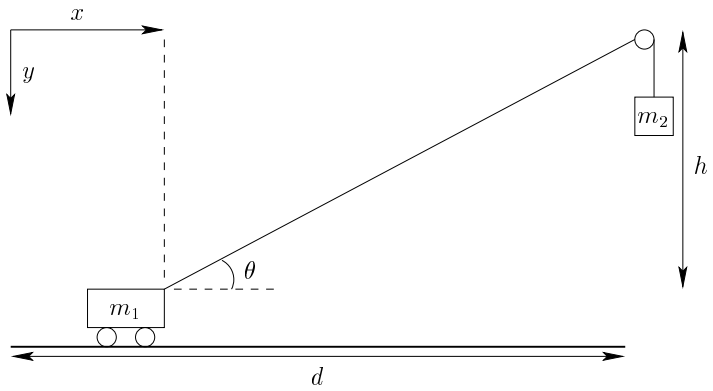


Figure 1.4: A cart of mass m_1 moves on a horizontal track under a variable force.

Solution We evaluate the angle θ from geometry,

$$\cos\theta = \frac{d-x}{\sqrt{(d-x)^2+h^2}}. \tag{1.22}$$

Because the angle varies with time, the force acting on m_1 likewise varies. Let the tension of the string be T; Newton's second law for m_1 is

$$T\cos\theta = m_1\ddot{x}, \tag{1.23}$$

and for m_2 is

$$m_2 g - T = m_2\ddot{y}, \tag{1.24}$$

where the dot accents denote derivatives with respective to time,

$$\dot{x} \equiv \frac{d}{dt}x(t), \quad \ddot{x} \equiv \frac{d^2}{dt^2}x(t).$$

We adopt this notation in succeeding chapters.

The length l of the string is constant, which imposes a constraint,

$$\sqrt{(d-x)^2+h^2}+y=l.$$

We thus express y and its derivatives in terms of x,

$$\dot{y}=\frac{d-x}{\sqrt{(d-x)^2+h^2}}\dot{x},$$

$$\ddot{y}=\frac{d-x}{\sqrt{(d-x)^2+h^2}}\ddot{x}-\frac{h^2}{[(d-x)^2+h^2]^{3/2}}\dot{x}^2.$$

Eliminating T from equations (1.23) and (1.24), we obtain

$$\frac{m_1\ddot{x}}{\cos\theta}+m_2\ddot{y}=m_2g.$$

Substituting $\cos\theta$ and $\ddot{y}$ with the above results, we form a second-order differential equation governing the motion of m_1,

$$\left[\frac{\sqrt{(d-x)^2+h^2}}{d-x}m_1+\frac{d-x}{\sqrt{(d-x)^2+h^2}}m_2\right]\ddot{x}-\frac{h^2}{[(d-x)^2+h^2]^{3/2}}m_2\dot{x}^2-m_2g=0, \tag{1.25}$$

for which the initial conditions are

$$x(0)=0,\quad \dot{x}(0)=0.$$

As this differential equation describing a simple situation has no analytic solution, we must resort to a numerical method in order to solve it.

Worksheet 1.9 The significance of names in the worksheet should be evident: `l` denotes l, and `y` denotes y. We find the second derivative of y, and assign it to another name `ddy`. We can type the differential equation, for which we have already a convenient shorthand notation `ddy` that we have just assigned for $\ddot{y}$. A command to arrange the terms in the equation is `collect`. To find a numerical solution of an equation, we must provide each parameter with a numerical value, such as mass, height, gravitational acceleration, etc., using the `eval` command. Then applying the `dsolve` command with the `numeric` option, we find the solution. Maple's output of a numerical solution is a procedure that provides a numerical value of x at any value of t.

```
> l := sqrt(d^2 + h^2);
```

$$l := \sqrt{d^2+h^2}$$

```
> y := l - sqrt((d-x(t))^2 + h^2);
```

$$y := \sqrt{d^2+h^2}-\sqrt{(d-\mathrm{x}(t))^2+h^2}$$

```
> dy := diff(y, t);
```

$$dy := \frac{(d-\mathrm{x}(t))\,(\frac{d}{dt}\mathrm{x}(t))}{\sqrt{(d-\mathrm{x}(t))^2+h^2}}$$

```
> ddy := diff(y, t$2);
```

$$ddy := \frac{(d-\mathrm{x}(t))^2\,(\frac{d}{dt}\mathrm{x}(t))^2}{((d-\mathrm{x}(t))^2+h^2)^{(3/2)}} - \frac{(\frac{d}{dt}\mathrm{x}(t))^2}{\sqrt{(d-\mathrm{x}(t))^2+h^2}} + \frac{(d-\mathrm{x}(t))\,(\frac{d^2}{dt^2}\mathrm{x}(t))}{\sqrt{(d-\mathrm{x}(t))^2+h^2}}$$

```
> Eq1 := m1*diff(x(t),t$2)*sqrt((d-x(t))^2+h^2)/(d-x(t)) + m2*ddy =
> m2*g;
```

$$Eq1 := \frac{m1\,(\frac{d^2}{dt^2}\mathrm{x}(t))\,\sqrt{\%1}}{d-\mathrm{x}(t)} + m2\left(\frac{(d-\mathrm{x}(t))^2\,(\frac{d}{dt}\mathrm{x}(t))^2}{\%1^{(3/2)}} - \frac{(\frac{d}{dt}\mathrm{x}(t))^2}{\sqrt{\%1}} + \frac{(d-\mathrm{x}(t))\,(\frac{d^2}{dt^2}\mathrm{x}(t))}{\sqrt{\%1}}\right) = m2\,g$$

$$\%1 := (d-\mathrm{x}(t))^2+h^2$$

```
> Eq2 := collect(Eq1, diff);
```

$$Eq2 := \left(\frac{m1\,\sqrt{\%1}}{d-\mathrm{x}(t)} + \frac{m2\,(d-\mathrm{x}(t))}{\sqrt{\%1}}\right)\left(\frac{d^2}{dt^2}\mathrm{x}(t)\right) + m2\left(\frac{(d-\mathrm{x}(t))^2}{\%1^{(3/2)}} - \frac{1}{\sqrt{\%1}}\right)\left(\frac{d}{dt}\mathrm{x}(t)\right)^2 = m2\,g$$

$$\%1 := (d-\mathrm{x}(t))^2+h^2$$

```
> Eq3 := eval(Eq2, {m1=0.5, m2=.05, d=1.5, h=0.5, g=9.8});
```

$$Eq3 := \left(\frac{0.5\,\sqrt{\%1}}{1.5-\mathrm{x}(t)} + \frac{0.05\,(1.5-\mathrm{x}(t))}{\sqrt{\%1}}\right)\left(\frac{d^2}{dt^2}\mathrm{x}(t)\right) + 0.05\left(\frac{(1.5-\mathrm{x}(t))^2}{\%1^{(3/2)}} - \frac{1}{\sqrt{\%1}}\right)\left(\frac{d}{dt}\mathrm{x}(t)\right)^2 = 0.490$$

$$\%1 := (1.5-\mathrm{x}(t))^2+0.25$$

```
> Eq4 := dsolve({Eq3, x(0)=0, D(x)(0)=0}, x(t), numeric);
```

$$Eq4 := \mathbf{proc}(x_rkf45)\ \ldots\ \mathbf{end\ proc}$$

```
> Eq4(0.3);
```

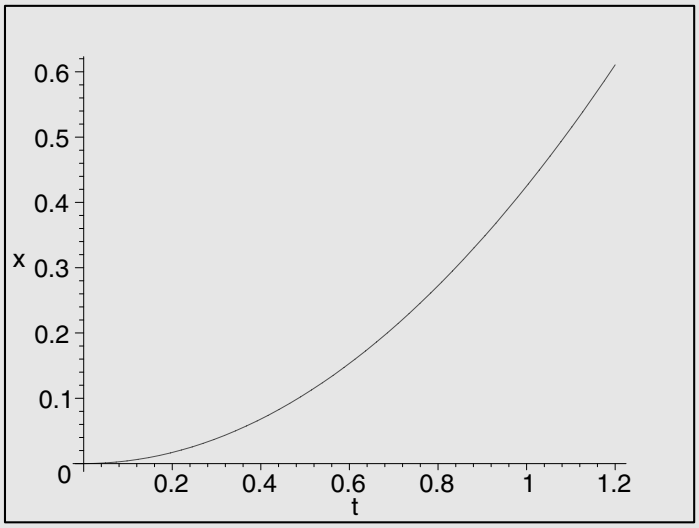
$$[t = 0.3,\ \mathrm{x}(t) = 0.0383714136584611329,\ \tfrac{d}{dt}\mathrm{x}(t) = 0.255734795915910474]$$

```
> Eq4(1.1);
```

$$[t = 1.1,\ \mathrm{x}(t) = 0.513698937324709281,\ \tfrac{d}{dt}\mathrm{x}(t) = 0.928984803649962832]$$

```
> with(plots):
Warning, the name changecoords has been redefined
```

```
> odeplot(Eq4, [t, x(t)], 0..1.2);
```



Maple has a large library of packages containing specialized commands; to use a command from such a package, one employs the `with` command to load the package. In the above example, we use the `odeplot` command which is contained in the `plots` package. With this command we plot the result of the numerical solution, which is a procedure, of a differential equation. (In preceding worksheets we plot an explicit function with the `plot` command, which is inapplicable in this situation.) One can invoke help to discover further information about any Maple usage.

1.5 Vectors and Matrices

Many physical quantities are vectors, which have both magnitude and direction. Maple provides the `LinearAlgebra` package to facilitate manipulations of vectors and matrices; in earlier versions of Maple, the `linalg` package served for this purpose. In Maple 8, a new package `VectorCalculus` is introduced; with the combination of `LinearAlgebra` and `VectorCalculus`, most tasks involving vector and matrix operations, as well as vector calculus, can be accomplished. In this book we avoid use of the `linalg` package; we will use the `LinearAlgebra` package extensively in our treatment of electromagnetism and relativity. Here we offer a few examples to demonstrate basic operations.

Example 1.6 We discuss projectile motion under a constant gravitational field. Newton's second law in vector form is

$$\mathbf{F} = m\mathbf{a}. \tag{1.26}$$

We choose the coordinate system such that the y direction is vertical with the positive sense upward. The equations of motion are thus

$$m\ddot{x} = 0, \quad m\ddot{y} = -mg,$$

and their integration are components of the position vector:

$$x = v_{0x}t, \quad y = v_{0y}t - \frac{1}{2}gt^2.$$

We consider an inclined plane that makes an angle α with the horizon; a projectile is launched from the bottom of the incline with speed v_0 in a direction making an angle β with the horizon, as shown in Figure 1.5. (a) Find the range R, which is the distance from the origin to the position at which the projectile lands on the plane. (b) Find the maximum value of the range.

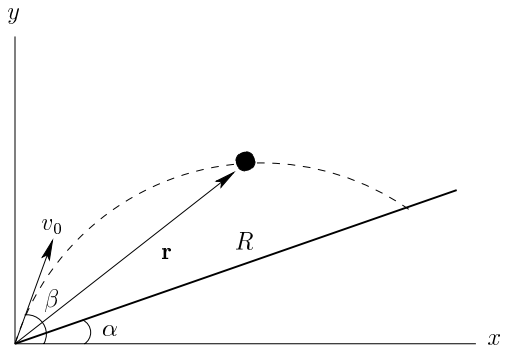


Figure 1.5: Shooting a projectile uphill.

Solution The position vector of the projectile is a function of time,

$$\mathbf{r} = (v_0 \cos\beta)t\,\hat{\mathbf{x}} + \left[(v_0 \sin\beta)t - \frac{1}{2}gt^2\right]\,\hat{\mathbf{y}},$$

where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit vectors along the coordinate axes. The position vector of a point on the incline is

$$\mathbf{s} = x\,\hat{\mathbf{x}} + x\tan\alpha\,\hat{\mathbf{y}}.$$

Landing occurs at a time and position at which the trajectory of the projectile and the inclined plane intersect, $\mathbf{r} = \mathbf{s}$. We require the solution of equations

$$(v_0 \cos\beta)t = x, \quad (v_0 \sin\beta)t - \frac{1}{2}gt^2 = x\tan\alpha.$$

We again apply Maple's `solve` command.

Worksheet 1.10 We activate the `LinearAlgebra` package by means of the `with` command. Because we work with trigonometric functions, we must provide Maple with information about our domain of interest. We apply the `assume` command to indicate the range of α and β; we also employ the `additionally` command to impose a further condition on a name to which is already attached an assumption. To choose items from lists or sequences, we use `[n]`, where n identifies the position of the desired element; for example, with `Eq1[2]` we choose the second solution. We use the `assign` command, which converts an equality sign `=` in the solution set into an assignment sign `:=`, so that we can call the names directly. The `simplify` command appears in various places, for obvious purposes.

```
> with(LinearAlgebra):
> assume(alpha>0, beta>0); additionally(alpha<Pi/2, beta<Pi/2);
additionally(beta>alpha);
> r := < v0*cos(beta)*t | v0*sin(beta)*t-1/2*g*t^2>;
```

$$r := \left[v0\cos(\beta)\,t,\ v0\sin(\beta)\,t - \frac{g\,t^2}{2}\right]$$

```
> s := < x | x*tan(alpha) >;
```

$$s := [x,\ x\tan(\alpha)]$$

```
> Eq1 := solve({r[1]=s[1], r[2]=s[2]},{x,t});
```

$$Eq1 := \{x = 0,\ t = 0\},$$
$$\left\{x = \frac{2\,v0^2\cos(\beta)\,(\sin(\beta) - \cos(\beta)\tan(\alpha))}{g},\ t = \frac{2\,v0\,(\sin(\beta) - \cos(\beta)\tan(\alpha))}{g}\right\}$$

```
> assign(Eq1[2]);
> t; x;
```

$$\frac{2\,v0\,(\sin(\beta) - \cos(\beta)\tan(\alpha))}{g}$$
$$\frac{2\,v0^2\cos(\beta)\,(\sin(\beta) - \cos(\beta)\tan(\alpha))}{g}$$

```
> R := x/cos(alpha);
```

$$R := \frac{2\,v0^2\cos(\beta)\,(\sin(\beta) - \cos(\beta)\tan(\alpha))}{g\cos(\alpha)}$$

```
> R := simplify(R);
```

$$R := -\frac{2\,v0^2\cos(\beta)\,(-\sin(\beta)\cos(\alpha) + \cos(\beta)\sin(\alpha))}{\cos(\alpha)^2\,g}$$

```
> dR := diff(R,beta);
```

$$dR := \frac{2\,v0^2\sin(\beta)\,(-\sin(\beta)\cos(\alpha) + \cos(\beta)\sin(\alpha))}{\cos(\alpha)^2\,g}$$
$$- \frac{2\,v0^2\cos(\beta)\,(-\cos(\beta)\cos(\alpha) - \sin(\beta)\sin(\alpha))}{\cos(\alpha)^2\,g}$$

```
> Eq12 := solve({dR=0}, {beta});
```

$$Eq12 := \{\beta = \arctan(\tan(\alpha) + \sqrt{\tan(\alpha)^2 + 1})\}, \{\beta = -\arctan(-\tan(\alpha) + \sqrt{\tan(\alpha)^2 + 1})\}$$

```
> Rmax := eval(R, Eq12[1]);
```

$$Rmax := -\frac{2\,v0^2\left(-\frac{\%1\cos(\alpha)}{\sqrt{1+\%1^2}} + \frac{\sin(\alpha)}{\sqrt{1+\%1^2}}\right)}{\sqrt{1+\%1^2}\cos(\alpha)^2\,g}$$

$$\%1 := \tan(\alpha) + \sqrt{\tan(\alpha)^2 + 1}$$

```
> Rmax := simplify(Rmax);
```

$$Rmax := \frac{v0^2}{(\sin(\alpha)+1)\,g}$$

We find

$$t = 2\frac{v_0(\sin\beta - \cos\beta\tan\alpha)}{g}, \quad x = 2\frac{v_0^2\cos\beta(\sin\beta - \cos\beta\tan\alpha)}{g},$$

and

$$R = 2\frac{v_0^2\cos\beta(\sin\beta - \cos\beta\tan\alpha)}{g\cos\alpha}.$$

The `simplify` command transforms R into

$$R = 2\frac{v_0^2\cos\beta(\sin\beta - \cos\beta\tan\alpha)}{g\cos\alpha} = 2\frac{v_0^2\cos\beta(\sin\beta\cos\alpha - \cos\beta\sin\alpha)}{g\cos^2\alpha},$$

but we can further simplify this expression. The angle sum relation for sine is

$$\sin(\beta - \alpha) = \sin\beta\cos\alpha - \sin\alpha\cos\beta.$$

We manually obtain a simplified result for R:

$$R = 2\frac{v_0^2\cos\beta\sin(\beta - \alpha)}{g\cos^2\alpha}.$$

Maple has powerful methods for simplifying expressions, but the definition of a "simplified" form varies from situation to situation and from user to user. One can force Maple to perform the above manipulations, but it is easier to do them manually. On many occasions in this book we discover that an optimally expressed result is obtained from a combination of computer and manual calculations.

To find the maximum range, we differentiate R with respect to β, and solve for β,

$$\frac{dR}{d\beta} = 0,$$

then substitute this value of β into R. Although the expression for β appears ugly,

$$\beta = \arctan(\tan\alpha + \sqrt{\tan^2\alpha + 1}),$$

Maple's `simplify` command produces an elegant final result for R:

$$R_{\text{max}} = \frac{v_0^2}{g(\sin\alpha + 1)}.$$

The above example can be regarded merely as writing a system of equations in a more compact notation. We use the following example to demonstrate a basic vector operation – the dot product.

Example 1.7 For some problems, spherical coordinates are superior to Cartesian coordinates. The relations between Cartesian coordinates (x, y, z) and spherical coordinates (r, θ, ϕ) are

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta. \tag{1.27}$$

The kinetic energy expressed in Cartesian coordinates is

$$T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2). \tag{1.28}$$

We seek the expression of kinetic energy in spherical coordinates.

Solution The kinetic energy is calculated as a dot product of the velocity vector with itself,

$$T = \frac{1}{2}m\,\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}. \tag{1.29}$$

We write the position vector as

$$\mathbf{r} = r\sin\theta\cos\phi\,\hat{\mathbf{x}} + r\sin\theta\sin\phi\,\hat{\mathbf{y}} + r\cos\theta\,\hat{\mathbf{z}}, \tag{1.30}$$

and perform the calculation with Maple.

Worksheet 1.11 We must explicitly specify that (r, θ, ϕ) are functions of time by typing `r(t)`, `theta(t)` and `phi(t)`. The `map` command applies operator `diff` to each component of the vector. Once `LinearAlgebra` is loaded, we can perform a scalar product by simply using the dot (`.`); alternatively, the `DotProduct(v, v)` command accomplishes the same task. A line over an expression denotes the complex conjugate. We first apply the `evalc` command, which is a symbolic evaluator over the complex field, and then the `simplify` command to the result, to achieve an optimal form.

```
> with(LinearAlgebra):

> x := < r(t)*sin(theta(t))*cos(phi(t)) |
> r(t)*sin(theta(t))*sin(phi(t)) | r(t)*cos(theta(t)) >;
```

$$x := [\mathrm{r}(t)\sin(\theta(t))\cos(\phi(t)),\ \mathrm{r}(t)\sin(\theta(t))\sin(\phi(t)),\ \mathrm{r}(t)\cos(\theta(t))]$$

```
> v := map(diff, x, t);
```

$$v := \left[(\tfrac{d}{dt}\,\mathrm{r}(t))\sin(\theta(t))\cos(\phi(t)) + \mathrm{r}(t)\cos(\theta(t))\,(\tfrac{d}{dt}\,\theta(t))\cos(\phi(t)) \right.$$
$$-\mathrm{r}(t)\sin(\theta(t))\sin(\phi(t))\,(\tfrac{d}{dt}\,\phi(t)),$$
$$(\tfrac{d}{dt}\,\mathrm{r}(t))\sin(\theta(t))\sin(\phi(t)) + \mathrm{r}(t)\cos(\theta(t))\,(\tfrac{d}{dt}\,\theta(t))\sin(\phi(t))$$
$$+\mathrm{r}(t)\sin(\theta(t))\cos(\phi(t))\,(\tfrac{d}{dt}\,\phi(t)),$$
$$\left.(\tfrac{d}{dt}\,\mathrm{r}(t))\cos(\theta(t)) - \mathrm{r}(t)\sin(\theta(t))\,(\tfrac{d}{dt}\,\theta(t))\right]$$

```
> vsq := v.v;
```

$$vsq := \overline{\Big((\tfrac{d}{dt}\,\mathrm{r}(t))\sin(\theta(t))\cos(\phi(t)) + \mathrm{r}(t)\cos(\theta(t))\,(\tfrac{d}{dt}\,\theta(t))\cos(\phi(t))} \setminus$$
$$\overline{-\mathrm{r}(t)\sin(\theta(t))\sin(\phi(t))\,(\tfrac{d}{dt}\,\phi(t))\Big)}$$
$$\Big((\tfrac{d}{dt}\,\mathrm{r}(t))\sin(\theta(t))\cos(\phi(t)) + \mathrm{r}(t)\cos(\theta(t))\,(\tfrac{d}{dt}\,\theta(t))\cos(\phi(t))$$
$$-\mathrm{r}(t)\sin(\theta(t))\sin(\phi(t))\,(\tfrac{d}{dt}\,\phi(t))\Big)$$
$$+$$
$$\overline{\Big((\tfrac{d}{dt}\,\mathrm{r}(t))\sin(\theta(t))\sin(\phi(t)) + \mathrm{r}(t)\cos(\theta(t))\,(\tfrac{d}{dt}\,\theta(t))\sin(\phi(t))} \setminus$$
$$\overline{+\mathrm{r}(t)\sin(\theta(t))\cos(\phi(t))\,(\tfrac{d}{dt}\,\phi(t))\Big)}$$
$$\Big((\tfrac{d}{dt}\,\mathrm{r}(t))\sin(\theta(t))\sin(\phi(t)) + \mathrm{r}(t)\cos(\theta(t))\,(\tfrac{d}{dt}\,\theta(t))\sin(\phi(t))$$
$$+\mathrm{r}(t)\sin(\theta(t))\cos(\phi(t))\,(\tfrac{d}{dt}\,\phi(t))\Big)$$
$$+\overline{\Big((\tfrac{d}{dt}\,\mathrm{r}(t))\cos(\theta(t)) - \mathrm{r}(t)\sin(\theta(t))\,(\tfrac{d}{dt}\,\theta(t))\Big)}\Big((\tfrac{d}{dt}\,\mathrm{r}(t))\cos(\theta(t))$$
$$-\mathrm{r}(t)\sin(\theta(t))\,(\tfrac{d}{dt}\,\theta(t))\Big)$$

```
> vsq := evalc(vsq);
```

$$vsq := \left(\left(\tfrac{d}{dt}\,\mathrm{r}(t)\right)\sin(\theta(t))\cos(\phi(t)) + \mathrm{r}(t)\cos(\theta(t))\left(\tfrac{d}{dt}\,\theta(t)\right)\cos(\phi(t)) - \mathrm{r}(t)\sin(\theta(t))\sin(\phi(t))\left(\tfrac{d}{dt}\,\phi(t)\right)\right)^2 + \left(\left(\tfrac{d}{dt}\,\mathrm{r}(t)\right)\sin(\theta(t))\sin(\phi(t)) + \mathrm{r}(t)\cos(\theta(t))\left(\tfrac{d}{dt}\,\theta(t)\right)\sin(\phi(t)) + \mathrm{r}(t)\sin(\theta(t))\cos(\phi(t))\left(\tfrac{d}{dt}\,\phi(t)\right)\right)^2 + \left(\left(\tfrac{d}{dt}\,\mathrm{r}(t)\right)\cos(\theta(t)) - \mathrm{r}(t)\sin(\theta(t))\left(\tfrac{d}{dt}\,\theta(t)\right)\right)^2$$

```
> vsq := simplify(vsq);
```

$$vsq := \mathrm{r}(t)^2\left(\tfrac{d}{dt}\,\phi(t)\right)^2 - \mathrm{r}(t)^2\left(\tfrac{d}{dt}\,\phi(t)\right)^2\cos(\theta(t))^2 + \left(\tfrac{d}{dt}\,\mathrm{r}(t)\right)^2 + \mathrm{r}(t)^2\left(\tfrac{d}{dt}\,\theta(t)\right)^2$$

This Maple worksheet shows that algebraic manipulation is considerable; we eventually obtain

$$\mathbf{v}\cdot\mathbf{v} = r^2\dot{\phi}^2 - r^2\dot{\phi}^2\cos^2\theta + \dot{r}^2 + r^2\dot{\theta}^2.$$

We combine the first two terms using the relation $1-\cos^2\theta = \sin^2\theta$, and obtain the kinetic energy as

$$T = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2). \tag{1.31}$$

Maple does not automatically simplify $1-\cos^2\theta = \sin^2\theta$; although one can make Maple do so, it is easier to do it manually. Here arises another instance of combining manual and computer calculations to produce an elegant final result.

Maple intrinsically assumes every variable to be complex. The general definition of the dot product involves a complex conjugate; explicitly,

$$\mathbf{v}\cdot\mathbf{v} = v_1^* v_1 + v_2^* v_2 + v_3^* v_3,$$

where the asterisk indicates the complex conjugate. A typical result of `simplify` is not the simplest form that we might desire, and a Maple user requires experience to instruct the software to produce a result nearest one's intent. The `evalc` command is useful when we have an expression that contains complex conjugates.

Matrix operations constitute the most important subject in linear algebra. There exist several books devoted exclusively to applying Maple to linear algebra. We use the following example to introduce diagonalization of a square matrix, which is a standard operation on a matrix. This topic is not crucially important for the rest of the book, and one need not panic if one

does not fully understand the underlying physics and the corresponding Maple commands. We merely provide the reader with an idea of the capability of the `LinearAlgebra` package for matrix operations.

Example 1.8 When we discuss the motion of a rigid body in space, we generally need to calculate the tensor of moments of inertia. At this point we can regard such a tensor simply as a 3 by 3 matrix,

$$\mathbf{I} = \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix}, \tag{1.32}$$

where the elements are

$$I_{xx} = \int \rho(y^2 + z^2)\, dV,$$

and

$$I_{yz} = \int \rho(-yz)\, dV,$$

and so on, with ρ as the mass density. According to a compact notation, in which occurs the Kronecker delta function ($\delta_{ij} = 1$ if $i = j$ and 0 otherwise),

$$I_{ij} = \int \rho(r^2 \delta_{ij} - r_i r_j)\, dV. \tag{1.33}$$

This matrix depends on the orientation of the chosen x, y and z axes. It is possible to find a particular orientation of a set of three mutually perpendicular axes such that, in this new coordinate system, matrix elements differ from zero only along the principal diagonal; these axes are called principal axes, and elements of the diagonal matrix are called the principal moments of inertia.

Find the tensor of moments of inertia of a uniform cube of side a taken about axes x, y, z coinciding with three intersecting edges of the cube, then diagonalize this matrix.

Solution The constant mass density is

$$\rho = \frac{M}{a^3}.$$

Directly from the definitions,

$$I_{xx} = \int_0^a \int_0^a \int_0^a \rho(y^2 + z^2)\, dx\, dy\, dz = \frac{2}{3} M a^2,$$

$$I_{yz} = \int_0^a \int_0^a \int_0^a \rho(-yz)\, dx\, dy\, dz = -\frac{1}{4} M a^2,$$

and so on. From direct evaluation of these integrals, we obtain

$$\mathbf{I} = \begin{pmatrix} \frac{2}{3}Ma^2 & -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 \end{pmatrix}. \tag{1.34}$$

To diagonalize a matrix, we find its eigenvalues I and eigenvectors $\mathbf{x}$, which satisfy

$$\mathbf{I}\mathbf{x} = I\mathbf{x}. \tag{1.35}$$

The eigenvalues are roots of the determinant

$$\det \begin{vmatrix} \frac{2}{3}Ma^2 - I & -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 - I & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 - I \end{vmatrix} = 0, \tag{1.36}$$

which generates a cubic equation in I. Because $\mathbf{I}$ is symmetric, we have three real roots I_1, I_2 and I_3. Maple has an integrated command to find eigenvalues and eigenvectors.

Worksheet 1.12 We perform triple integration as a nested structure. This worksheet involves sophisticated operations on vectors, but most are rarely needed in our future chapters. We leave it to the reader to discover further information from help under `?LinearAlgebra`. The `Eigenvectors` command computes the eigenvectors. We select the matrix elements using `[n, m]`. The `Normalize` command normalizes a vector so that its inner product with itself is unity. The `CrossProduct` command evaluates the vector product of two vectors. Matrix multiplication can be performed with a dot (`.`) within the `LinearAlgebra` command.

```
> rho := M/(a*a*a);
```

$$\rho := \frac{M}{a^3}$$

```
> Ixx := int(int(int(rho*(y^2+z^2), x=0..a), y=0..a), z=0..a);
```

$$Ixx := \frac{2\,M\,a^2}{3}$$

```
> Iyy := int(int(int(rho*(x^2+z^2), x=0..a), y=0..a), z=0..a);
```

$$Iyy := \frac{2\,M\,a^2}{3}$$

```
> Izz := int(int(int(rho*(x^2+y^2), x=0..a), y=0..a), z=0..a);
```

$$Izz := \frac{2\,M\,a^2}{3}$$

```
> Ixy := int(int(int(rho*(-x*y), x=0..a), y=0..a) ,z=0..a);
```

$$Ixy := -\frac{M\,a^2}{4}$$

```
> Ixz := int(int(int(rho*(-x*z), x=0..a), y=0..a), z=0..a);
```

$$Ixz := -\frac{M\,a^2}{4}$$

```
> Iyz := int(int(int(rho*(-y*z), x=0..a), y=0..a), z=0..a);
```

$$Iyz := -\frac{M\,a^2}{4}$$

```
> Iyx := Ixy;
```

$$Iyx := -\frac{M\,a^2}{4}$$

```
> Izx := Ixz;
```

$$Izx := -\frac{M\,a^2}{4}$$

```
> Izy := Iyz;
```

$$Izy := -\frac{M\,a^2}{4}$$

```
> with(LinearAlgebra):
> In := <<Ixx | Ixy | Ixz>, <Iyx | Iyy | Iyz>, <Izx | Izy | Izz>>;
```

$$In := \begin{bmatrix} \frac{2\,M\,a^2}{3} & -\frac{M\,a^2}{4} & -\frac{M\,a^2}{4} \\ -\frac{M\,a^2}{4} & \frac{2\,M\,a^2}{3} & -\frac{M\,a^2}{4} \\ -\frac{M\,a^2}{4} & -\frac{M\,a^2}{4} & \frac{2\,M\,a^2}{3} \end{bmatrix}$$

```
> (lam, vec) := Eigenvectors(In);
```

$$lam,\ vec := \begin{bmatrix} \frac{M\,a^2}{6} \\ \frac{11\,M\,a^2}{12} \\ \frac{11\,M\,a^2}{12} \end{bmatrix}, \begin{bmatrix} 1 & -1 & -1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$$

```
> v1 := vec[1..3, 1];
```

$$v1 := \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

```
> v1 := Normalize(v1, 2);
```

$$v1 := \begin{bmatrix} \frac{\sqrt{3}}{3} \\ \frac{\sqrt{3}}{3} \\ \frac{\sqrt{3}}{3} \end{bmatrix}$$

```
> v3 := vec[1..3, 3];
```

$$v3 := \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$

```
> v3 := Normalize(v3, 2);
```

$$v3 := \begin{bmatrix} -\frac{\sqrt{2}}{2} \\ 0 \\ \frac{\sqrt{2}}{2} \end{bmatrix}$$

```
> v2 := CrossProduct(v1, v3);
```

$$v2 := \begin{bmatrix} \frac{\sqrt{3}\sqrt{2}}{6} \\ -\frac{\sqrt{3}\sqrt{2}}{3} \\ \frac{\sqrt{3}\sqrt{2}}{6} \end{bmatrix}$$

```
> Rot := <v1 | v2 | v3>;
```

$$Rot := \begin{bmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}\sqrt{2}}{6} & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}\sqrt{2}}{3} & 0 \\ \frac{\sqrt{3}}{3} & \frac{\sqrt{3}\sqrt{2}}{6} & \frac{\sqrt{2}}{2} \end{bmatrix}$$

```
> Prin := Transpose(Rot).In.Rot;
```

$$Prin := \begin{bmatrix} \frac{M\,a^2}{6} & 0 & 0 \\ 0 & \frac{11\,M\,a^2}{12} & 0 \\ 0 & 0 & \frac{11\,M\,a^2}{12} \end{bmatrix}$$

From the output of the `Eigenvectors` command, we find three sets of vectors that satisfy

$$\begin{pmatrix} \frac{2}{3}Ma^2 & -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{6}Ma^2 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix},$$

$$\begin{pmatrix} \frac{2}{3}Ma^2 & -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 \end{pmatrix} \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} = \frac{11}{12}Ma^2 \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix},$$

$$\begin{pmatrix} \frac{2}{3}Ma^2 & -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 \end{pmatrix} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} = \frac{11}{12}Ma^2 \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}.$$

We thus obtain three principal moments of inertia, two of them equal:

$$I_1 = \frac{1}{6}Ma^2, \quad I_2 = I_3 = \frac{11}{12}Ma^2.$$

The normalized principal axis associated with I_1 is the first eigenvector divided by the square root of its inner product, $\sqrt{1^2 + 1^2 + 1^2} = \sqrt{3}$,

$$\begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix},$$

which specifies the body diagonal of the cube. Because I_2 and I_3 are repeated roots, their associated principal axes are two mutually perpendicular vectors in a plane perpendicular to I_1. As Maple provides a pair of vectors that are not mutually perpendicular, we must make a construction for this purpose. We choose the third principal axis to be

$$\begin{pmatrix} \frac{-1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix},$$

so that the second principal axis can be constructed as the cross-product of the other two:

$$\begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{-2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{pmatrix}.$$

We form a matrix $\mathbf{R}$ of which columns are the eigenvectors of $\mathbf{I}$. We form a transposed matrix $\tilde{\mathbf{R}}$, which simply converts columns of $\mathbf{R}$ into rows, and make the following calculation,

$$\tilde{\mathbf{R}}\mathbf{I}\mathbf{R},$$

which is called the similarity transformation. We obtain a matrix with diagonal elements only:

$$\begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{-1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{2}{3}Ma^2 & -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 & -\frac{1}{4}Ma^2 \\ -\frac{1}{4}Ma^2 & -\frac{1}{4}Ma^2 & \frac{2}{3}Ma^2 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{-2}{\sqrt{6}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{6}Ma^2 & 0 & 0 \\ 0 & \frac{11}{12}Ma^2 & 0 \\ 0 & 0 & \frac{11}{12}Ma^2 \end{pmatrix}.$$

1.6 Summary

Here follows a list of Maple commands that we have encountered in this chapter.

```
arccos    additionally  assign  assume  assuming  BesselJ
BesselY   collect       cos     csc     D         diff
dsolve    eval          evalc   evalf   exp       expand
int       map           Pi      plot    plot3d    restart
rhs       simplify      sin     solve   subs      sqrt
```

Mastering these commands allows us to overcome many predicaments that we experience in every problem in physics, from basic arithmetic to sophisticated integral; for this reason it is important to understand their functional purpose and the context of their usage. Take the utmost advantage of the help facility, which provides many examples; moreover, help on one command typically prompts "see also" which gives related commands for further exploration.

We invoke the `plots` package, which contains `odeplot`; we also call the `LinearAlgebra` package, which contains these commands.

```
CrossProduct  DotProduct  Eigenvectors  Normalize  Transpose
```

These are basic tasks in linear algebra, and we will discuss them extensively in the chapters on electromagnetism and relativity.

Exercises

1. Type `?Pi` in a Maple input line, and read the help text. Notice that `gamma` is pre-defined as Euler's constant; any attempt to use it for another purpose (e.g., Lorentz factor γ) will result in error.

2. Find the roots to a generic cubic equation
$$ax^3 + bx^2 + cx + d = 0. \tag{1.37}$$

3. Find the solution of a system of three linear equations
$$\begin{cases} a_1x + b_1y + c_1z = d_1, \\ a_2x + b_2y + c_2z = d_2, \\ a_3x + b_3y + c_3z = d_3. \end{cases} \tag{1.38}$$

4. Essentially all integrals listed in standard mathematical tables can be performed with Maple. For example, evaluate the following integrals:
$$\int \frac{1}{x^2 + a^2}\,dx, \quad \int \frac{x}{(a + bx)(c + dx)}\,dx, \quad \int \frac{x^2}{c^3 \pm x^3}\,dx.$$

Discover more examples so as to become confident in the use of Maple to evaluate integrals.

5. Verify that

$$\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2}\,dx = \sqrt{2\pi}.$$

A physicist claims that "believe it or not, a significant fraction of the theoretical physics literature consists of performing variations and elaborations of this basic Gaussian integral."[4] For $a > 0$, evaluate the following integrals in his book:

$$\int_{-\infty}^{\infty} e^{-\frac{1}{2}ax^2}\,dx, \quad \int_{-\infty}^{\infty} e^{-\frac{1}{2}ax^2+Jx}\,dx, \quad \int_{-\infty}^{\infty} e^{-\frac{1}{2}ax^2+iJx}\,dx;$$

the `assume` command is necessary.

6. Most differential equations in textbooks on this subject can be solved with Maple. Discover differential equations in your past or current textbook to verify this statement. For example, find the general solution of this system of first-order linear equations:

$$\begin{cases} \dot{x}_1 = x_1 + x_2 + x_3, \\ \dot{x}_2 = 2x_1 + x_2 - x_3, \\ \dot{x}_3 = -8x_1 - 5x_2 - 3x_3. \end{cases}$$

Multiple equations in a set are accepted in the `dsolve` command analogous to the syntax in `solve`.

7. From experiment one obtains a rule of collision for two particles moving in one dimension,

$$v_{1f} - v_{2f} = -\epsilon(v_{1i} - v_{2i}), \tag{1.39}$$

where ϵ is called the coefficient of restitution. This coefficient, ranging from 0 to 1, is a measure of the loss of energy at a collision: if $\epsilon = 1$, a collision is elastic; if $\epsilon = 0$, the two particles move with the same velocity, as if they have become amalgamated. Using this rule of collision, and conservation of momentum, find the velocities of the particles after collision. Verify that, when $\epsilon = 1$, one obtains the result of elastic collision as in equation (1.6).

8. The motion of a rocket projected vertically upward in a uniform gravitational field is described by an equation

$$(m_0 - \alpha t)\frac{d}{dt}v(t) - \alpha v_e = -(m_0 - \alpha t)g, \tag{1.40}$$

where v_e is the velocity of the exhausted gases relative to the rocket, m_0 is the initial mass, and α is the rate of loss of mass, all assumed to be constant. If the rocket begins

[4] A. Zee, *Quantum Field Theory in a Nutshell*, Princeton, NJ: Princeton University Press, 2003, p. 13.

from rest at time $t = 0$, that is $v(0) = 0$, solve the differential equation with Maple. Verify that, with further manual arrangement of the Maple output, the velocity is

$$v(t) = -gt + v_e \ln\left(\frac{m_0}{m_0 - \alpha t}\right). \tag{1.41}$$

Assuming $v_e = 2072.6$ m s^{-1} and α to be $1/60$ s^{-1} of the initial mass, plot the velocity from $t = 0$ to $t = 55$ s.

9. Employ the `Eigenvectors` command in the `LinearAlgebra` package to find all eigenvalues and eigenvectors of this matrix:

$$\begin{pmatrix} 3 & 2 & 2 \\ 1 & 4 & 1 \\ -2 & -4 & -1 \end{pmatrix}.$$

10. For every chapter in this book, the most important exercise is to apply Maple to the solution of problems, which one might discover in various textbooks. Among the infinite possibilities of doing so, we provide an example of the use of Maple to perform calculations that appear in *Feynman Lectures* vol. 3.

    (a) Find eigenvalues of the following matrices:

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{12} & H_{22} \end{pmatrix}, \quad \begin{pmatrix} A & 0 & 0 & 0 \\ 0 & -A & 2A & 0 \\ 0 & 2A & -A & 0 \\ 0 & 0 & 0 & A \end{pmatrix},$$

    which are Hamiltonian matrices taken from p. 9-6 in explaining the ammonia maser, and p. 12-6 in explaining the "21-centimeter line" of hydrogen.

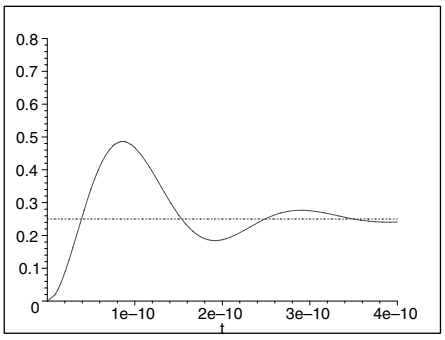


Figure 1.6: The absolute square of C_- in equation (1.44).

(b) On p. 11–17, there is a system of differential equations:

$$\begin{aligned} i\frac{dC_+}{dt} &= \omega_0 C_+ + AC_- + AC_+, \\ i\frac{dC_-}{dt} &= \omega_0 C_- + AC_+ + AC_-, \end{aligned} \tag{1.42}$$

where $i = \sqrt{-1}$ and $A = (\alpha - i\beta)/2$ (both α and β are real). With initial conditions $C_+(0) = 1$ and $C_-(0) = 0$, prove that the solution for $C_-(t)$ is

$$C_- = \frac{1}{2} e^{-i\omega_0 t}(e^{-\beta t} e^{-i\alpha t} - 1). \tag{1.43}$$

The absolute square of C_- is

$$|C_-|^2 = \frac{1}{4}[1 + e^{-2\beta t} - 2e^{-\beta t}\cos(\alpha t)], \tag{1.44}$$

although proof of this condition requires a command `conjugate` not discussed in this chapter. Plot equation (1.44), with $\alpha = \pi \times 10^{10}$ s^{-1} and $\beta = 10^{10}$ s^{-1}, which should resemble Figure 1.6; as a test, make another plot with these values: $\alpha = 4\pi \times 10^{10}$ s^{-1} and $\beta = 10^{10}$ s^{-1}. Feynman used this plot to introduce a fascinating quantum system consisting of neutral K mesons.[5]

[5]For the reader interested in particle physics, see D. H. Perkins, *Introduction to High Energy Physics*, 4th ed., New York: Cambridge University Press, 1999, p. 230; to produce a plot based on experimental data, use $\beta = (2\ \tau_S)^{-1}$ and $\alpha = \Delta m$, where $\tau_S = 0.89 \times 10^{-10}$ s is the lifetime of K_S^0 and $\Delta m = 0.53 \times 10^{10}$ s^{-1} (with $c = \hbar = 1$) is the mass difference between K_L^0 and K_S^0.

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2 Oscillatory Motion

Second-order differential equations with constant coefficients serve as mathematical models for important physical processes, such as the motion of a spring-mass system, and oscillating electric circuits. Mathematically this type of problems involve comparing undetermined coefficients, and Maple can conveniently solve them symbolically and numerically. We use the capability of Maple to solve differential equations to investigate an important subject in mechanics – oscillatory motion.

2.1 Simple Harmonic Oscillator

An object of mass m is attached at the end of a spring; the spring exerts a restoring force proportional to a displacement x from its equilibrium position. We write this force as $-kx$, where k is the force constant (or spring constant). According to Newton's second law, the equation of motion is

$$m\ddot{x} = -kx. \tag{2.1}$$

We solve this equation directly with Maple's `dsolve` command.

Worksheet 2.1

```
> dsolve(m*diff(x(t),t$2) + k*x(t) = 0, x(t));
```

$$\mathrm{x}(t) = _C1 \sin\left(\frac{\sqrt{k}\,t}{\sqrt{m}}\right) + _C2 \cos\left(\frac{\sqrt{k}\,t}{\sqrt{m}}\right)$$

In the Maple output, the general solution is

$$x = C_1 \sin\left(\sqrt{\frac{k}{m}}\,t\right) + C_2 \cos\left(\sqrt{\frac{k}{m}}\,t\right). \tag{2.2}$$

The angular frequency is hence

$$\omega_0 = \sqrt{\frac{k}{m}}, \tag{2.3}$$

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ISBN: 3-527-40640-9

and we write the solution as

$$x = C_1 \sin(\omega_0 t) + C_2 \cos(\omega_0 t). \tag{2.4}$$

If the initial displacement and initial velocity are supplied, both coefficients C_1 and C_2 can be determined.

Example 2.1 Suppose that an object of mass 5.0 kg stretches a spring 0.01 m. If the object is displaced an additional 0.01 m, and is then set in motion with an initial velocity 0.3 m s^{-1}, determine the equation of motion.

Solution The force constant is calculated as

$$(5.0 \text{ kg})(9.8 \text{ m s}^{-2}) = (k)\ (0.01 \text{ m}), \quad k = 4900 \text{ N m}^{-1}.$$

The differential equation and associated initial conditions are

$$5.0\ddot{x} + 4900x = 0, \quad x(0) = 0.01, \quad \dot{x}(0) = 0.3.$$

Providing this information to the `dsolve` command, we obtain the solution

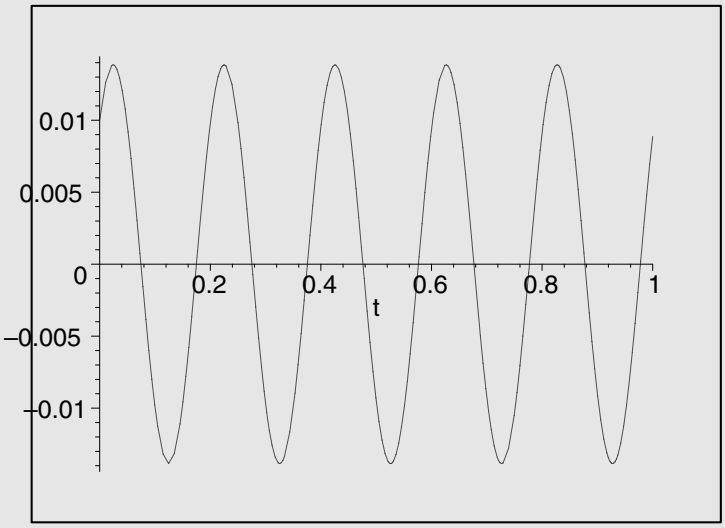
$$x = \frac{3\sqrt{5}}{700} \sin(14\sqrt{5}\, t) + \frac{1}{100} \cos(14\sqrt{5}\, t).$$

Worksheet 2.2 If we provide a differential equation with initial conditions as a set (enclosed within braces) to the `dsolve` command, Maple returns the result without undetermined coefficients.

```
> Soln1 := dsolve({5*diff(x(t),t$2) + 4900*x(t) = 0, x(0)=.01,
> D(x)(0)=.3}, x(t));
```

$$Soln1 := \mathrm{x}(t) = \frac{3}{700} \sin(14\sqrt{5}\, t)\sqrt{5} + \frac{1}{100} \cos(14\sqrt{5}\, t)$$

```
> plot(rhs(Soln1), t=0..1);
```



A simple harmonic oscillator is governed by a restoring force that is linear with respect to the displacement from the equilibrium position, for instance, $-kx$ in the spring-mass system. Most oscillating systems are governed by a more complicated restoring force. If the displacement from the equilibrium position is small, we can approximate the force as being proportional to the displacement. A function $f(x)$ can generally be expanded about $x = a$ as a Taylor series:

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \frac{(x-a)^3}{3!}f'''(a) + \ldots + \frac{(x-a)^n}{n!}f^{(n)}(a) + \ldots. \quad (2.5)$$

If $x - a$ is small, we can retain only the linear term so that $f(x)$ becomes a linear function.

We use the following example to illustrate this approximation of a small oscillation.

Example 2.2 Two identical charges $+q$ fixed in space are separated by a distance d. A third charge $-Q$ of mass m is free to move and lies initially at rest on the perpendicular bisector of the two fixed charges. Show that, with a displacement x small compared with d, the third charge $-Q$ undergoes simple harmonic motion along the perpendicular bisector.

Solution From Figure 2.1, the distance r between $-Q$ and either $+q$ is

$$r = \sqrt{\left(\frac{d}{2}\right)^2 + x^2}.$$

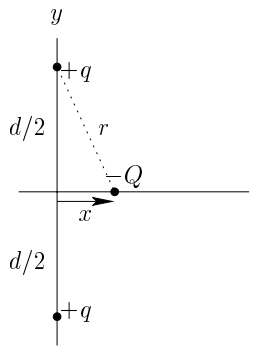


Figure 2.1: Configuration of three charges.

According to Coulomb's law (see Section 6.1), the x component of the force that charge $-Q$ experiences is

$$F = -2\frac{kqQ}{r^2}\frac{x}{r},$$

where x/r is the cosine of the angle between r and the x axis. For small x, we can expand F about $x = 0$ to obtain

$$F = -\frac{16kqQ}{d^3}x + \frac{96kqQ}{d^5}x^3 - \frac{480kqQ}{d^7}x^5 + \ldots,$$

and retain only the linear term. We obtain the equation of motion for charge $-Q$:

$$m\ddot{x} = -\frac{16kqQ}{d^3}x,$$

which has the same form as for a simple harmonic oscillator. The angular frequency is then identified as

$$\omega_0 = \sqrt{\frac{16kqQ}{md^3}}.$$

Worksheet 2.3 In this worksheet we introduce the `taylor` command, which forms an expansion as a Taylor series. We use the `convert` command to convert the result of that series expansion to a polynomial, specified by the `polynom` option.

```
> assume(d>0):
> r := ((d/2)^2+x^2)^(1/2);
```

$$r := \sqrt{\frac{d^2}{4} + x^2}$$

```
> F := -2*k*q*Q/r^2*x/r;
```

$$F := -\frac{2\,k\,q\,Q\,x}{\left(\frac{d^2}{4}+x^2\right)^{(3/2)}}$$

```
> taylor(F, x=0);
```

$$-\frac{16\,k\,q\,Q}{d^3}\,x+\frac{96\,k\,q\,Q}{d^5}\,x^3-\frac{480\,k\,q\,Q}{d^7}\,x^5+\mathrm{O}(x^7)$$

```
> convert(%, polynom);
```

$$-\frac{16\,k\,q\,Q\,x}{d^3}+\frac{96\,k\,q\,Q\,x^3}{d^5}-\frac{480\,k\,q\,Q\,x^5}{d^7}$$

Practically any binding force can be approximated as a linear restoring force for sufficiently small displacement from equilibrium, and the force constant k is the first derivative of the force evaluated at equilibrium.

2.2 Damped Oscillation

For a real oscillator, the amplitude of oscillation gradually diminishes as a consequence of the existence of a damping force. An approximation commonly employed for this damping force is

$$F_d = b\dot{x}, \tag{2.6}$$

so that force F_d is proportional to the velocity, with b as the damping coefficient. We modify the equation governing the spring-mass system by adding this extra component for a more realistic situation,

$$m\ddot{x} + b\dot{x} + kx = 0. \tag{2.7}$$

We again submit this equation directly to the `dsolve` command to obtain

$$x = C_1 e^{-\frac{b-\sqrt{b^2-4km}}{2m}t} + C_2 e^{-\frac{b+\sqrt{b^2-4km}}{2m}t}. \tag{2.8}$$

Worksheet 2.4

```
> dsolve(m*diff(x(t),t$2) + b*diff(x(t),t) + k*x(t) = 0, x(t));
```

$$\mathrm{x}(t) = _C1\; e^{(\frac{(-b+\sqrt{b^2-4\,k\,m})\,t}{2\,m})} + _C2\; e^{(-\frac{(b+\sqrt{b^2-4\,k\,m})\,t}{2\,m})}$$

Based on the sign of $b^2 - 4mk$, we classify the solution as:

1. overdamping, for which $b^2 > 4mk$,
2. underdamping, for which $b^2 < 4mk$, and
3. critical damping, for which $b^2 = 4mk$,

which we treat separately.

2.2.1 Overdamping

If $b^2 > 4mk$, the solution is written as

$$x = C_1 e^{-\frac{b-\sqrt{b^2-4km}}{2m}t} + C_2 e^{-\frac{-b+\sqrt{b^2-4km}}{2m}t}. \tag{2.8}$$

To evaluate C_1 and C_2, we apply the initial conditions in order to solve for these coefficients. This task can be directly accomplished with `dsolve` if we provide the initial conditions.

Example 2.3 A block attached to a spring and moving through a viscous material serves as an example of overdamped motion. Suppose that we have such a mechanical system governed by a differential equation[1]

$$\ddot{x} + 1.2\dot{x} + 0.25x = 0.$$

Find the solution for initial conditions in two cases:
(a) $x(0) = 0.5, \dot{x}(0) = 1.75$;
(b) $x(0) = 0.5, \dot{x}(0) = -1.75$.

Solution Maple produces these solutions.
(a)

$$x = 3.3e^{-0.27t} - 2.8e^{-0.93t}.$$

(b)

$$x = -1.9e^{-0.27t} + 2.4e^{-0.93t}.$$

Worksheet 2.5 The usage of `dsolve` is straightforward. At the end we convert fractions into decimals with the `evalf` command: after all, most physical quantities are measured in decimals.

[1] Many differential equations in this chapter are taken from Boyce and Diprima 2001, § 3.8 and § 3.9.

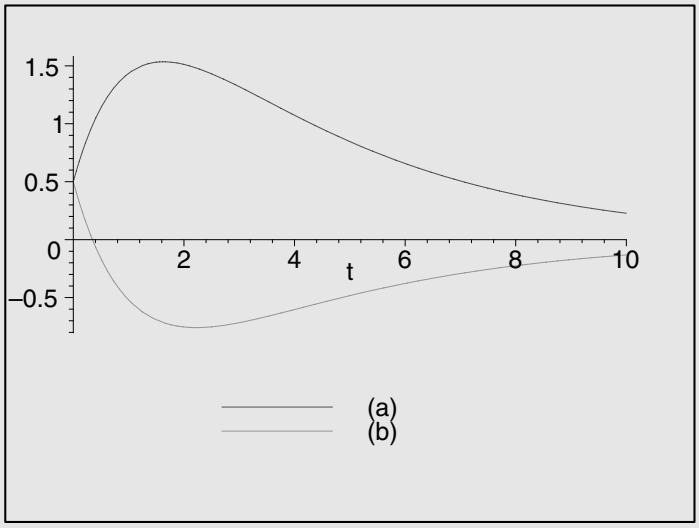
```
> Soln4 := dsolve({diff(x(t),t$2) + 1.2*diff(x(t),t) + 0.25*x(t) =
0,
> x(0)=0.5, D(x)(0)=1.75}, x(t));
```

$$Soln4 := \mathrm{x}(t) = \left(\frac{1}{4} + \frac{41\sqrt{11}}{44}\right) e^{(\frac{(-6+\sqrt{11})\,t}{10})} + \left(-\frac{41\sqrt{11}}{44} + \frac{1}{4}\right) e^{(-\frac{(6+\sqrt{11})\,t}{10})}$$

```
> Soln5 := dsolve({diff(x(t),t$2) + 1.2*diff(x(t),t) + 0.25*x(t) =
0,
> x(0)=0.5, D(x)(0)=-1.75}, x(t));
```

$$Soln5 := \mathrm{x}(t) = \left(\frac{1}{4} - \frac{29\sqrt{11}}{44}\right) e^{(\frac{(-6+\sqrt{11})\,t}{10})} + \left(\frac{29\sqrt{11}}{44} + \frac{1}{4}\right) e^{(-\frac{(6+\sqrt{11})\,t}{10})}$$

```
> plot([rhs(Soln4), rhs(Soln5)], t=0..10, legend=["(a)", "(b)"]);
```




```
> evalf(Soln4); evalf(Soln5);
```

$$\mathrm{x}(t) = 3.340491282\, e^{(-0.2683375210\,t)} - 2.840491282\, e^{(-0.9316624790\,t)}$$

$$\mathrm{x}(t) = -1.935957248\, e^{(-0.2683375210\,t)} + 2.435957248\, e^{(-0.9316624790\,t)}$$

In (a), the block has a positive velocity and at first moves away from the equilibrium position. In (b), it has a negative initial velocity, and it moves toward then across zero, the equilibrium position. In both cases, the block eventually returns to zero displacement with an exponential decay.

2.2.2 Underdamping

In this situation, it is convenient to use Euler's formula,

$$e^{i\theta} = \cos\theta + i\sin\theta, \tag{2.9}$$

to rearrange the equation. The solution becomes

$$x = e^{-\frac{bt}{2m}}\left[A\cos\left(\frac{\sqrt{4km-b^2}}{2m}t\right) + B\sin\left(\frac{\sqrt{4km-b^2}}{2m}t\right)\right], \tag{2.10}$$

where A and B are linear combinations of C_1 and C_2. We define a quantity ω_q as the quasi-frequency,

$$\omega_\mathrm{q} = \frac{\sqrt{4km-b^2}}{2m}. \tag{2.11}$$

When $b = 0$, the quasi-frequency is

$$\omega_0 = \sqrt{\frac{k}{m}},$$

which corresponds to the angular frequency of a simple harmonic oscillator. We generally call ω_0 the natural frequency.

From given initial conditions, we can also evaluate numerically the two coefficients A and B.

Example 2.4 An object of mass 1.0 kg is attached to a spring of force constant 1.0 N m^{-1}; the damping coefficient is 0.125 kg s^{-1}; the initial displacement is 2.0 m, and initial velocity 0.

Solution The object is governed by this equation:

$$\ddot{x} + 0.125\dot{x} + x = 0, \quad x(0) = 2, \quad \dot{x}(0) = 0.$$

For comparison, we write an equation without damping, that is with $b = 0$:

$$\ddot{x} + x = 0, \quad x(0) = 2, \quad \dot{x}(0) = 0.$$

As before, we employ the `dsolve` command to find the solutions, which are

$$\begin{aligned} &x = 2\cos t, && \text{without damping,}\\ &x = 2e^{-0.625t}\cos(0.998t) + 0.125e^{-0.625t}\sin(0.998t), && \text{with damping.}\end{aligned}$$

The solution for damped oscillation differs from that for undamped oscillation in incorporating an exponential decay; we also observe that the quasi-frequency ω_q is 0.998 s^{-1}, slightly different from the natural frequency $\omega_0 = 1.0$ s^{-1} for the undamped case.

Worksheet 2.6 Although Maple gives a generic solution of $m\ddot{x} + b\dot{x} + kx = 0$ in terms of exponential functions, when we provide the values of m, b and k such that $b^2 < 4mk$, Maple returns the solution in terms of sinusoidal functions.

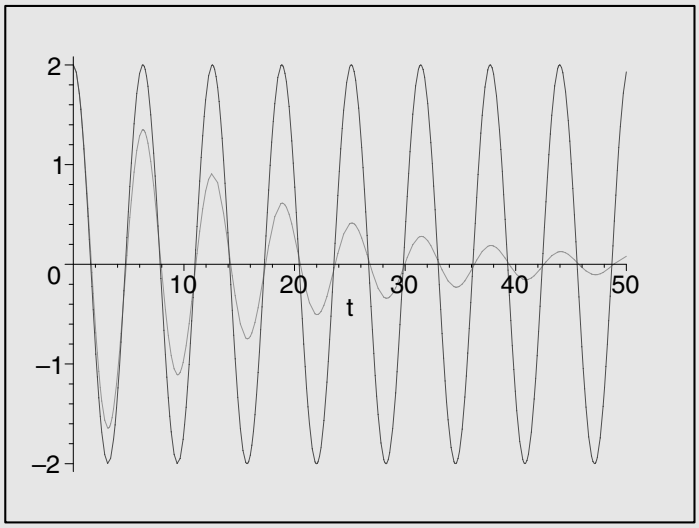
```
> Soln7 := dsolve({diff(x(t),t$2) + x(t) = 0, x(0)=2, D(x)(0)=0},
> x(t));
```

$$Soln7 := \mathrm{x}(t) = 2\cos(t)$$

```
> Soln8 := dsolve({diff(x(t),t$2) + 0.125*diff(x(t),t) + x(t) = 0,
> x(0)=2, D(x)(0)=0}, x(t));
```

$$Soln8 := \mathrm{x}(t) = \frac{2}{255}\sqrt{255}\,e^{(-\frac{t}{16})}\sin\left(\frac{\sqrt{255}\,t}{16}\right) + 2\,e^{(-\frac{t}{16})}\cos\left(\frac{\sqrt{255}\,t}{16}\right)$$

```
> plot([rhs(Soln7), rhs(Soln8)], t=0..50);
```




```
> evalf(Soln7); evalf(Soln8);
```

$$\mathrm{x}(t) = 2.\cos(t)$$

$$\mathrm{x}(t) = 0.1252448582\,e^{(-0.06250000000\,t)}\sin(0.9980449638\,t) + 2.\,e^{(-0.06250000000\,t)}\cos(0.9980449638\,t)$$

2.2.3 Critical Damping

One rarely encounters a situation of critical damping, because such an exact mathematical equality does not occur in a physical situation: a measurement is necessarily made for slightly greater or less than the critical value. The mathematical structure of the solution in this situation differs from the other cases. Because the root of the quadratic equation is repeated,

another independent solution is required. The general solution takes a form

$$x = C_1 e^{-\frac{b}{2m}t} + C_2 t e^{-\frac{b}{2m}t}. \tag{2.12}$$

Example 2.5 Find solutions of the differential equation

$$\ddot{x} + \dot{x} + 0.25x = 0, \quad x(0) = 0.5, \quad \dot{x}(0) = 1.75.$$

Solution A calculation with Maple yields

$$x = \frac{1}{2}e^{-t/2} + 2t\, e^{-t/2},$$

which is consistent with the general form of critical damping.

Worksheet 2.7 Maple can discern the situation of critical damping and give two independent solutions correctly.

```
> Soln10 := dsolve({diff(x(t),t$2) + 1.0*diff(x(t),t) + 0.25*x(t)
> = 0, x(0)=0.5, D(x)(0)=1.75}, x(t));
```

$$Soln10 := \mathrm{x}(t) = \frac{1}{2}\, e^{(-\frac{t}{2})} + 2\, e^{(-\frac{t}{2})}\, t$$

We leave it as an exercise for the reader to make a plot of the above solution.

2.3 Sinusoidally Driven Oscillation

Before discussing the physics of a driven oscillation, we digress to explore some Maple commands that are useful in further study.

Example 2.6 We pose the following problems to introduce Maple commands that are helpful for our next topic.

1. A function is defined as

   $$f(x) = x^2 + 1.$$

   Evaluate $f(5)$.

2. The expression $A\cos(\omega t) + B\sin(\omega t)$ can be written as $C\cos(\omega t - \delta)$; find C and δ in terms of A and B.

Solution For the first problem, we know how to assign an expression to a name, using the operator `:=`. To evaluate x^2+1 at $x = 5$, we can employ the `eval` command, but this operation is inconvenient for multiple evaluations of the same expression. In the following worksheet we introduce both an arrow notation `->` and the `unapply` command, either of which enables us to define our own functions.

For the second problem, we have observed the phenomenon that adding two sinusoidal functions of the same frequency results in another sinusoidal function, of the same frequency, but different amplitude and phase. For instance, in the example in Section 2.1, the solution

$$x = 0.01\cos(31.3\,t) + 0.0096\sin(31.3\,t)$$

is equivalent to

$$x = 0.14\cos(31.3\,t - 0.76).$$

One can verify this result using the trigonometric addition formula, or directly from the graph.

In general, we can combine two sinusoidal functions of the same frequency to become one function,

$$A\cos(\omega t) + B\sin(\omega t) = C\cos(\omega t - \delta), \tag{2.13a}$$

where

$$C = \sqrt{A^2 + B^2}, \quad \delta = \arctan\frac{B}{A}. \tag{2.13b}$$

Worksheet 2.8 We assign the expression $x^2 + 1$ to a name `y`, and evaluate `y` at $x = 5$ using the `eval` command. We try to define the function using `f(x) := x^2 + 1;`, but this operation is unsuccessful. This line merely assigns the expression to a name `f(x)`; when we type `f(5)` this symbol is interpreted as a separate name. To define a function, we require an important command: the arrow notation, shown for our definition of `g`, produces the desired effect. We define a function alternatively using the `unapply` command, as in our usage for `h`. For the trigonometric equation, we employ a rather tricky combination of the `expand` and `identity` commands to solve for C and δ.

```
> y := x^2 + 1;
```

$$y := x^2 + 1$$

```
> eval(y, x=5);
```

$$26$$

```
> f(x) := x^2 + 1;
```

$$\mathrm{f}(x) := x^2 + 1$$

```
> f(5);
```

$$\mathrm{f}(5)$$

```
> g := x -> x^2 + 1;
```

$$g := x \to x^2 + 1$$

```
> g(5);
```

$$26$$

```
> h := unapply(y, x);
```

$$h := x \to x^2 + 1$$

```
> h(5);
```

$$26$$

```
> solve(identity(A*cos(alpha*t) + B*sin(alpha*t) =
> expand(C*cos(alpha*t-delta)), t), {C, delta});
```

$$\left\{C = \sqrt{B^2 + A^2},\ \delta = \arctan\left(\frac{B}{\sqrt{B^2 + A^2}},\ \frac{A}{\sqrt{B^2 + A^2}}\right)\right\},$$
$$\left\{C = -\sqrt{B^2 + A^2},\ \delta = \arctan\left(-\frac{B}{\sqrt{B^2 + A^2}},\ -\frac{A}{\sqrt{B^2 + A^2}}\right)\right\}$$

```
> solve(identity(0.01*cos(31.3*t) + 0.0096*sin(31.3*t) =
> expand(C*cos(31.3*t-delta)), t), {C, delta});
```

$$\{C = -0.01386217876,\ \delta = -2.376599821\},\ \{\delta = 0.7649928327,\ C = 0.01386217876\}$$

Here we return to physics. If we apply a periodic external force to a spring-mass system, the situation is called forced oscillation or driven oscillation. The differential equation governing this system is that of damped oscillation with an additional sinusoidal function,

$$m\ddot{x} + b\dot{x} + kx = F_0 \cos(\omega t). \tag{2.14}$$

We distinguish two types of frequencies in such a problem. The driving frequency is denoted by ω, which is typically a controllable variable: using a motor to drive the motion, we can vary ω by adjusting the speed of rotation. The natural frequency is denoted as

$$\omega_0 = \sqrt{\frac{k}{m}},$$

which is the same definition as for the simple harmonic oscillator; this natural frequency is determined once we have chosen the mass and the spring with its particular force constant.

This type of differential equation can be solved analytically. To illustrate the forced response, here is an example with three distinct driving frequencies.

Example 2.7 For the equation,

$$\ddot{x} + 0.125\dot{x} + x = F(t), \quad x(0) = 2, \quad \dot{x}(0) = 0,$$

plot the solution $x(t)$ and $F(t)$ for the following driving forces:

(a) $F(t) = 3\cos(0.3t)$; (b) $F(t) = 3\cos(t)$; (c) $F(t) = 3\cos(3t)$.

Observe the relation between amplitude and phase of the force and the solution.

Solution The natural frequency is

$$\omega_0 = \sqrt{\frac{k}{m}} = 1.0.$$

The three forces represent situations when the driving frequency is (a) less than, (b) equal to, and (c) greater than, the natural frequency. The solutions for the three driving frequencies are

(a) $x = -0.12e^{-0.0625t}\sin(0.998t) - 1.29e^{-0.0625t}\cos(0.998t) + 0.14\sin(0.3t) + 3.3\cos(0.3t)$,

(b) $x = -23.9e^{-0.0625t}\sin(0.998t) + 2.0e^{-0.0625t}\cos(0.998t) + 24.0\sin(t)$,

(c) $x = 0.096e^{-0.0625t}\sin(0.998t) + 2.37e^{-0.0625t}\cos(0.998t) + 0.018\sin(3t) - 0.37\cos(3t)$.

Worksheet 2.9 This worksheet illustrates that Maple's `dsolve` command works for nonhomogeneous differential equations as well.

```
> Epr1 := diff(x(t),t$2) + 0.125*diff(x(t),t) + x(t);
```

$$Epr1 := \left(\frac{d^2}{dt^2}\,\mathrm{x}(t)\right) + 0.125\left(\frac{d}{dt}\,\mathrm{x}(t)\right) + \mathrm{x}(t)$$

```
> F1:=3*cos(0.3*t);
```

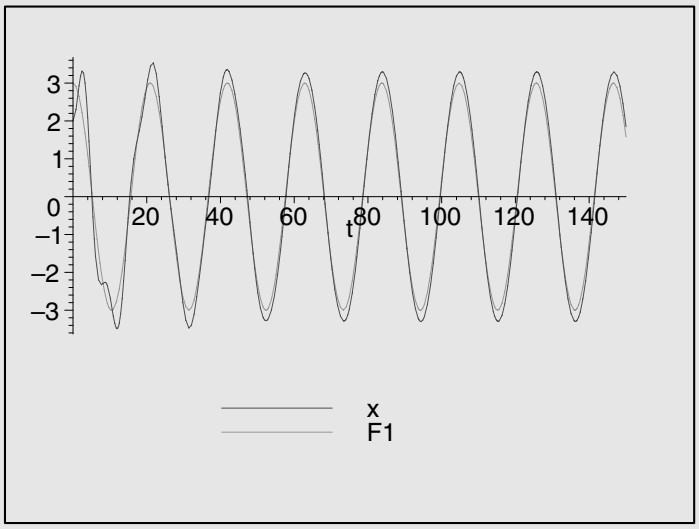
$$F1 := 3\cos(0.3\,t)$$

```
> Soln11 := dsolve({Epr1 = F1, x(0)=2, D(x)(0)=0}, x(t));
```

$$Soln11 := \mathrm{x}(t) = -\frac{257758}{33843855}\,e^{\left(-\frac{t}{16}\right)}\sin\left(\frac{\sqrt{255}\,t}{16}\right)\sqrt{255}$$

$$-\frac{171358}{132721}\,e^{\left(-\frac{t}{16}\right)}\cos\left(\frac{\sqrt{255}\,t}{16}\right) + \frac{18000}{132721}\sin\left(\frac{3\,t}{10}\right) + \frac{436800}{132721}\cos\left(\frac{3\,t}{10}\right)$$

```
> plot([rhs(Soln11), F1], t=0..150, legend=["x", "F1"]);
```



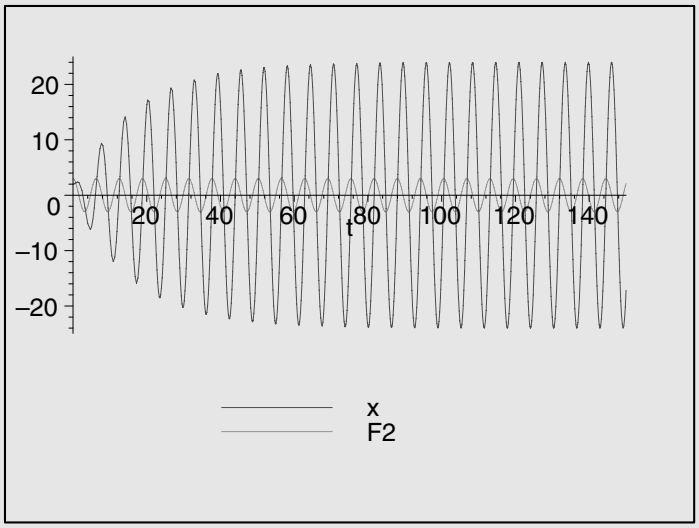

```
> F2 := 3*cos(t);
```

$$F2 := 3\cos(t)$$

```
> Soln13 := dsolve({Epr1 = F2, x(0)=2, D(x)(0)=0}, x(t));
```

$$Soln13 := \mathrm{x}(t) = -\frac{382}{255}\, e^{(-\frac{t}{16})} \sin\left(\frac{\sqrt{255}\, t}{16}\right) \sqrt{255} + 2\, e^{(-\frac{t}{16})} \cos\left(\frac{\sqrt{255}\, t}{16}\right) + 24\sin(t)$$

```
> plot([rhs(Soln13), F2], t=0..150, legend=["x", "F2"]);
```



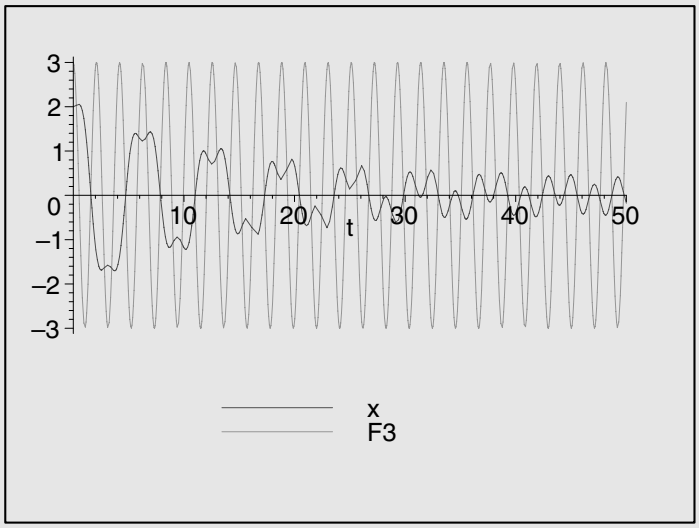
```
> F3 := 3*cos(3*t);
```

$$F3 := 3\cos(3\,t)$$

```
> Soln15 := dsolve({Epr1 = F3, x(0)=2, D(x)(0)=0}, x(t));
```

$$Soln15 := \mathrm{x}(t) = \frac{74}{12315}\,e^{(-\frac{t}{16})}\sin\left(\frac{\sqrt{255}\,t}{16}\right)\sqrt{255} + \frac{9746}{4105}\,e^{(-\frac{t}{16})}\cos\left(\frac{\sqrt{255}\,t}{16}\right) + \frac{72}{4105}\sin(3\,t) - \frac{1536}{4105}\cos(3\,t)$$

```
> plot([rhs(Soln15), F3], t=0..50, legend=["x", "F3"]);
```




```
> evalf(Soln11); evalf(Soln13); evalf(Soln15);
```

$$\mathrm{x}(t) = -0.1216192771\,e^{(-0.06250000000\,t)}\sin(0.9980449638\,t) - 1.291114443\,e^{(-0.06250000000\,t)}\cos(0.9980449638\,t) + 0.1356228479\sin(0.3000000000\,t) + 3.291114443\cos(0.3000000000\,t)$$

$$\mathrm{x}(t) = -23.92176792\,e^{(-0.06250000000\,t)}\sin(0.9980449638\,t) + 2.\,e^{(-0.06250000000\,t)}\cos(0.9980449638\,t) + 24.\sin(t)$$

$$\mathrm{x}(t) = 0.09595495227\,e^{(-0.06250000000\,t)}\sin(0.9980449638\,t) + 2.374177832\,e^{(-0.06250000000\,t)}\cos(0.9980449638\,t) + 0.01753958587\sin(3.\,t) - 0.3741778319\cos(3.\,t)$$

From the graphical output we observe that, in each case, after an initial irregular motion, the mass oscillates at the driving frequency ω with a constant amplitude. This stabilized sinusoidal curve is the force response; the amplitude and phase of the force response vary

according to ω. When ω is smaller than ω_0, the force response roughly follows the driving force, and they oscillate in phase. When ω is equal to the natural frequency ω_0, the response is extremely large, and the phase lags behind the driving force by $\pi/2$. When ω is larger than ω_0, the force response is small and it oscillates nearly out of phase (a phase difference of π) with the driving force.

According to the above results, the solution for driven oscillation has a general form:

$$x = e^{-\frac{bt}{2m}}\left[A_1\cos\left(\frac{\sqrt{4km-b^2}}{2m}t\right) + B_1\sin\left(\frac{\sqrt{4km-b^2}}{2m}t\right)\right] + C_3\sin(\omega t) + C_4\cos(\omega t). \tag{2.15}$$

The first two terms of the solution are called transient, because they diminish when t becomes large; they contribute to irregular motion at the beginning of oscillation. This transient is simply the general solution for a damped oscillation. The third and fourth terms constitute the steady-state solution, because they do not decay; they correspond to the force response. From our trials we have discovered that C_3 and C_4 depend on experimental conditions such as mass m, damping coefficient b, force constant k, and driving frequency ω, but not on the initial conditions x_0 and $\dot{x}_0$. To evaluate the amplitude, we write the sum of sine and cosine in this form:

$$C_3\sin(\omega t) + C_4\cos(\omega t) = A\cos(\omega t - \delta); \tag{2.16}$$

we already know how to express A and δ in terms of C_3 and C_4 from equation (2.13). A relation between amplitude and phase of the force and its response is thus derived. Using Maple to undertake the rearrangement, we have

$$A = \frac{F_0}{\sqrt{m^2(\omega^2-\omega_0^2)^2 + b^2\omega^2}}, \tag{2.17}$$

and

$$\delta = \tan^{-1}\frac{b\omega}{m(\omega_0^2-\omega^2)}. \tag{2.18}$$

Worksheet 2.10 To break an expression into parts, the `op` command is convenient. We extract the force response, which is the third part of `Epr3`, using `op(3, Epr3)`. We again adopt a combination of the `expand` and `identity` commands to find the amplitude and phase. Using the `assign` command, which turns `=` into `:=`, we can call `A` and `delta` directly. We require the `unapply` command to define the amplitude and phase as functions of b. Finally, we introduce Maple's operator `seq`, which generates a sequence of expressions; see `?seq` for additional information.

```
> Eq1 := m*diff(x(t),t$2) + b*diff(x(t),t) + m*omega0^2*x(t) =
> F0*cos(omega*t);
```

$$Eq1 := m\left(\frac{d^2}{dt^2}\,\mathrm{x}(t)\right) + b\left(\frac{d}{dt}\,\mathrm{x}(t)\right) + m\,\omega 0^2\,\mathrm{x}(t) = F0\cos(\omega\,t)$$

```
> Soln2 := dsolve(Eq1, x(t));
```

$$Soln2 := \mathrm{x}(t) = e^{\left(\frac{(-b+\sqrt{b^2-4\,\omega 0^2\,m^2})\,t}{2\,m}\right)}_C2 + e^{\left(-\frac{(b+\sqrt{b^2-4\,\omega 0^2\,m^2})\,t}{2\,m}\right)}_C1 + \frac{F0\,((m\,\omega 0^2-\omega^2\,m)\cos(\omega\,t)+\omega\sin(\omega\,t)\,b)}{\omega^4\,m^2+(b^2-2\,\omega 0^2\,m^2)\,\omega^2+\omega 0^4\,m^2}$$

```
> Epr3 := rhs(Soln2);
```

$$Epr3 := e^{\left(\frac{(-b+\sqrt{b^2-4\,\omega 0^2\,m^2})\,t}{2\,m}\right)}_C2 + e^{\left(-\frac{(b+\sqrt{b^2-4\,\omega 0^2\,m^2})\,t}{2\,m}\right)}_C1 + \frac{F0\,((m\,\omega 0^2-\omega^2\,m)\cos(\omega\,t)+\omega\sin(\omega\,t)\,b)}{\omega^4\,m^2+(b^2-2\,\omega 0^2\,m^2)\,\omega^2+\omega 0^4\,m^2}$$

```
> Epr4 := op(3, Epr3);
```

$$Epr4 := \frac{F0\,((m\,\omega 0^2-\omega^2\,m)\cos(\omega\,t)+\omega\sin(\omega\,t)\,b)}{\omega^4\,m^2+(b^2-2\,\omega 0^2\,m^2)\,\omega^2+\omega 0^4\,m^2}$$

```
> Soln5 := solve(identity(Epr4 = expand(A*cos(omega*t-delta)), t),
{A, delta});
```

$$Soln5 := \left\{A = \frac{F0}{\sqrt{\%1}},\ \delta = \arctan\left(\frac{\omega\,b}{\sqrt{\%1}},\ \frac{m\,(\omega 0^2-\omega^2)}{\sqrt{\%1}}\right)\right\},\ \left\{A = -\frac{F0}{\sqrt{\%1}},\ \delta = \arctan\left(-\frac{\omega\,b}{\sqrt{\%1}},\ -\frac{m\,(\omega 0^2-\omega^2)}{\sqrt{\%1}}\right)\right\}$$

$$\%1 := b^2\,\omega^2+\omega 0^4\,m^2-2\,\omega 0^2\,m^2\,\omega^2+\omega^4\,m^2$$

```
> assign(Soln5[1]);
```

```
> A; delta;
```

$$\frac{F0}{\sqrt{b^2\,\omega^2+\omega 0^4\,m^2-2\,\omega 0^2\,m^2\,\omega^2+\omega^4\,m^2}}$$

$$\arctan\left(\frac{\omega\,b}{\sqrt{b^2\,\omega^2+\omega 0^4\,m^2-2\,\omega 0^2\,m^2\,\omega^2+\omega^4\,m^2}},\ \frac{m\,(\omega 0^2-\omega^2)}{\sqrt{b^2\,\omega^2+\omega 0^4\,m^2-2\,\omega 0^2\,m^2\,\omega^2+\omega^4\,m^2}}\right)$$

```
> F0 := 1.0;  m := 1.0;  omega0 := 1.0;
```

$$F0 := 1.0$$
$$m := 1.0$$
$$\omega 0 := 1.0$$

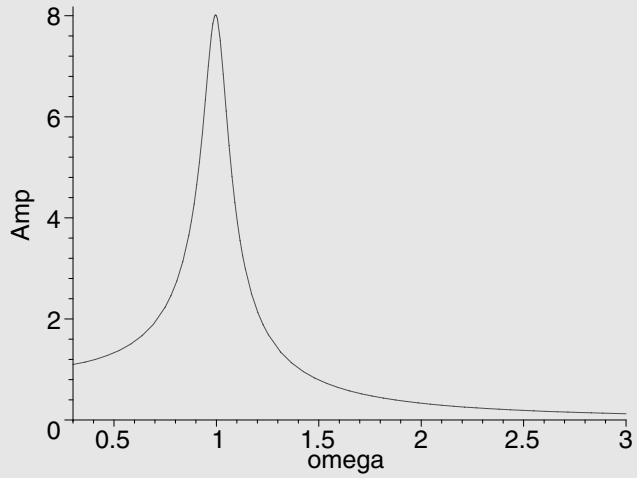
```
> Amp := unapply(A, b);
```

$$Amp := b \to \frac{1.0}{\sqrt{b^2\,\omega^2 + 1.000000 - 2.0000\,\omega^2 + 1.00\,\omega^4}}$$

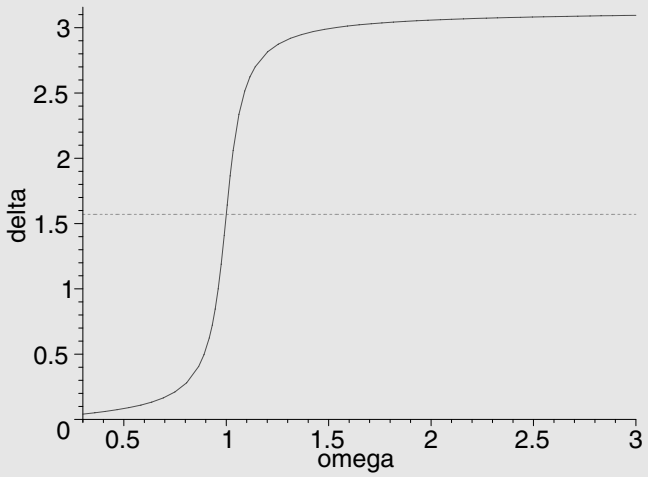
```
> pha := unapply(delta, b);
```

$$pha := b \to \arctan\left(\frac{\omega\, b}{\sqrt{b^2\,\omega^2 + 1.000000 - 2.0000\,\omega^2 + 1.00\,\omega^4}}, \frac{1.0\,(1.00 - \omega^2)}{\sqrt{b^2\,\omega^2 + 1.000000 - 2.0000\,\omega^2 + 1.00\,\omega^4}}\right)$$

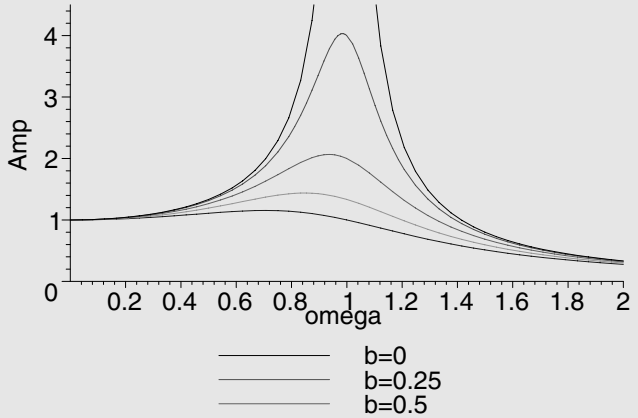
```
> plot(Amp(0.125), omega=0.3..3);
```



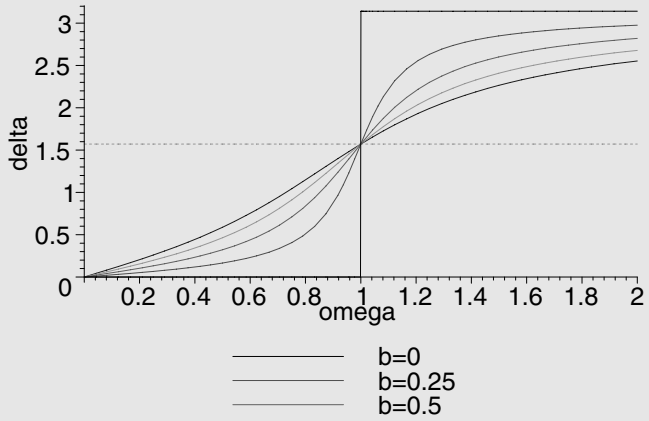
```
> plot([pha(0.125), Pi/2], omega=0.3..3);
```




```
> plot([seq(Amp(i/4), i=0..4)], omega=0..2, 0..4.5, legend=["b=0",
> "b=0.25", "b=0.5", "b=0.75", "b=1"]);
```



```
> plot([seq(pha(i/4), i=0..4), Pi/2], omega=0..2, legend=["b=0",
> "b=0.25", "b=0.5", "b=0.75", "b=1", "Pi/2"]);
```



For one specific value $b = 0.125$, we plot the amplitude and phase versus the driving frequency ω. These plots indicate that when $\omega = \omega_0$, the amplitude is large; this phenomenon is called resonance. At this frequency, the force response lags behind the driving force by $\pi/2$, as we have seen. The plot also indicates that, at small frequency, the force response and driving force are in phase; at large frequency, they are out of phase.

We plot curves of the force response with various damping coefficients b in a series. For small b, the response at resonance is much larger than the amplitude of the driving force. We also plot curves of phase angle in a sequence with various damping coefficients b; at resonance, the phase angle is $\pi/2$.

2.4 Phase Space

A second-order differential equation with constant coefficients is exactly solvable; it serves as a satisfactory model for many oscillatory systems, but for some situations this model is inadequate. For instance, to describe the motion of a pendulum in a gravitational field with a damping force, the angle x relative to the vertical is governed by an equation

$$ml^2\ddot{x} + bl\dot{x} + mgl\sin(x) = 0. \tag{2.19}$$

When x is small, we can make the small-angle approximation such that $\sin(x) \cong x$, and reduce it to the same equation of damped oscillation. For a large angle, it is difficult to write the solution.

As explained in the preceding chapter, most differential equations that we encounter in physics admit no analytic solution, even for simple systems. In subsequent chapters we rely strongly on numerical solutions, for which reason here we discuss numerical methods to solve differential equations. We also introduce a related topic, phase space, in which a dynamical system can be represented.

A second-order differential equation of this form

$$\frac{d^2x}{dt^2} + q(x)\frac{dx}{dt} = r(x) \tag{2.20}$$

can be reduced to two equations of first order:

$$\frac{dx}{dt} = v, \tag{2.21a}$$

$$\frac{dv}{dt} = r(x) - q(x)v \equiv f(x, v). \tag{2.21b}$$

For instance, we write the equation for the pendulum as two first-order differential equations:

$$\frac{dx}{dt} = v, \tag{2.22a}$$

$$\frac{dv}{dt} = -\frac{g}{l}\sin(x) - \frac{b}{ml}v. \tag{2.22b}$$

According to this approach we regard x and v as separate variables. Treating a variable and its derivative as separate dependent variables is an important concept in the calculus of variations and the Lagrangian formulation of mechanics, which we discuss in the next chapter.

If we have initial conditions, that is if x_0 and v_0 at time t_0 are given, we use these two first-order equations to integrate forwards in time, and obtain approximate values $(x_1, v_1), (x_2, v_2), \ldots, (x_n, v_n)$ at $t_n = t_0 + n\,\Delta t$. Using the Euler method as an illustrative example,

$$x_1 = x_0 + v_0\,\Delta t, \quad v_1 = v_0 + f(x_0, v_0)\,\Delta t,$$

$$x_2 = x_1 + v_1\,\Delta t, \quad v_2 = v_1 + f(x_1, v_1)\,\Delta t,$$

we advance to a subsequent time t_n,

$$x_n = x_{n-1} + v_{n-1}\,\Delta t, \quad v_n = v_{n-1} + f(x_{n-1}, v_{n-1})\,\Delta t. \tag{2.23}$$

Numerical solution conforms to this principle. The Euler method is merely a pedagogical model, which typically lacks sufficient accuracy. In practice the Runge–Kutta method is commonly used; we do not discuss this method here but the idea is the same as the Euler method.

There are many computer codes in existence to undertake calculations of numerical solutions to differential equations. Maple's `dsolve` command includes an option for numerical solution, which conveniently incorporates those routines in a simple line command.

We define a two-dimensional plane with coordinates of position x and velocity v as a *phase space*; in this phase space, each point (x, v) represents an instantaneous state. A second-order differential equation of the above form can be geometrically presented in such a phase space. At any point (x, v), we evaluate a slope as

$$\frac{dv}{dx} = \frac{\frac{dv}{dt}}{\frac{dx}{dt}} = \frac{f(x,v)}{v}.$$

We can draw a short arrow through the point (x, v) with this slope; a collection of all such arrows is called a *direction field*. It is a simple task for Maple to generate such a plot with the `DEtools` package.

Example 2.8 Suppose a pendulum to be governed by an equation

$$\ddot{x} + 0.2\dot{x} + \sin(x) = 0,$$

find the numerical solution with initial conditions

$$x(0) = \frac{\pi}{1.01}, \quad \dot{x}(0) = 0.$$

Solution We can numerically solve this equation. To produce a plot of the direction field, we must write the second-order equation as two first-order equations:

$$\begin{aligned} &\frac{dx}{dt} = v, \\ &\frac{dv}{dt} + 0.2v + \sin(x) = 0. \end{aligned}$$

Worksheet 2.11 We first invoke the `DEtools` and the `plots` packages. The differential equation is solved numerically using `dsolve` with an option `numeric`. To write the second-order equation as two first-order equations, we employ the `subs` commands to substitute $\dot{x}$ with v. The `dfieldplot` command produces the direction field, and the `odeplot` command graphs the numerical solution from `dsolve`, for both x versus t and x versus $\dot{x}$. We introduce the `display` command in the `plots` package to superpose two or more plots.

```
> with(plots): with(DEtools):
Warning, the name changecoords has been redefined
```

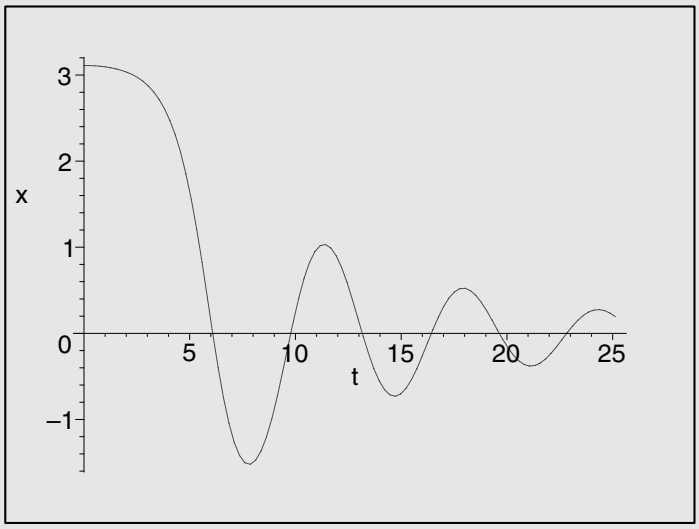
```
> Eq1 := diff(x(t), t$2) + 0.2*diff(x(t), t) + sin(x(t)) = 0;
```

$$Eq1 := (\frac{d^2}{dt^2}\,\mathrm{x}(t)) + 0.2\,(\frac{d}{dt}\,\mathrm{x}(t)) + \sin(\mathrm{x}(t)) = 0$$

```
> Soln2 := dsolve({Eq1, x(0)=Pi/1.01, D(x)(0)=0}, x(t), numeric);
```

$$Soln2 := \mathbf{proc}(x_rkf45) \ldots \mathbf{end\ proc}$$

```
> odeplot(Soln2, [t, x(t)], t=0..8*Pi, numpoints=100);
```




```
> Eq11 := diff(x(t), t) = v(t);
```

$$Eq11 := \frac{d}{dt}\,\mathrm{x}(t) = \mathrm{v}(t)$$

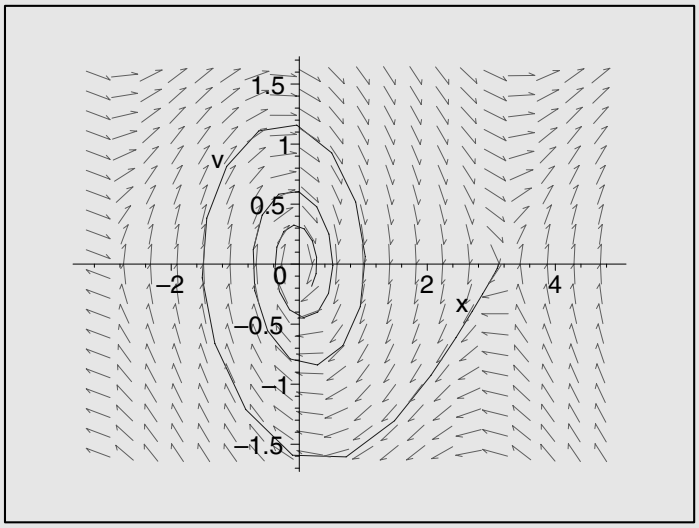
```
> Eq12 := subs(Eq11, Eq1);
```

$$Eq12 := (\frac{d}{dt}\,\mathrm{v}(t)) + 0.2\,\mathrm{v}(t) + \sin(\mathrm{x}(t)) = 0$$

```
> p1 := dfieldplot([Eq11, Eq12], [x(t), v(t)], t=0..8*Pi,
> x=-Pi..3/2*Pi, v=-Pi/2..Pi/2):

> p2 := odeplot(Soln2, [x(t), diff(x(t), t)], t=0..8*Pi,
> color=blue, thickness=2):
```

```
> display([p1, p2]);
```



According to this numerical solution, we plot the position (angle) x versus time t. To represent the solution in an alternative way, we plot the velocity $v = \dot{x}$ versus x, which gives a trajectory in the phase space. For an oscillatory system, representation of the solution as a trajectory in the phase space is generally superior, because it indicates a cyclic or chaotic property more markedly. In this example, the trajectory spirals into the center. A dynamic system can be classified according to the pattern of such a trajectory; this topic can be found in many books.

Superposing the trajectory and the direction field, we see that the trajectory traverses the phase space tangential to the direction arrows. A plot of direction field in phase space thus allows us to understand qualitative properties of differential equations.

In classical physics, we can in principle completely determine the motion of a particle if we are given the position and velocity at one instant with the governing differential equation. This view can be understood with the plot in the phase space. We mentioned above that each point (x, v) in the phase space represents a state, which is a possible initial condition. Tracing the arrows we can find its past and future.

However, no physical measurement can be given as an exact number. For the pendulum system, within the regime of small angle (small x), the arrows form a stable stream, in the neighborhood of $(\pi, 0)$ in phase; that is, if the pendulum is released nearly upright vertically, the trajectory might differ greatly for two similar initial conditions. In this situation, a minute variation of the initial state can result in a great variation at a subsequent stage. This sensitive dependence on initial conditions is one characteristic of a nonlinear dynamic system; see next example.

Example 2.9 An equation to describe the current x in a triode oscillator, called the van der Pol equation, is

$$\ddot{x} - \mu(1 - x^2)\dot{x} + x = 0, \tag{2.24}$$

where μ is a positive constant. Discuss the solution of this van der Pol equation at $\mu = 1$.

Solution We make a set of trajectories in the phase space, referred to as a *phase portrait*, using the `DEtools` package. In the phase space, there seems to exist a limit circle, which implies a stable periodic solution. Experimenting with numerical solutions, we discover that, if an initial condition is slightly less than $(2, 0.169)$, the trajectory completes almost one cycle then begins to sink into the center, whereas, if an initial condition is slightly greater than $(2, 0.169)$, the trajectory also completes almost one cycle but then drifts away. On the basis of these trials we conclude that a periodic solution exists with $x = 2$ and $0.168 < v < 0.170$. This example illustrates the sensitive dependence on initial conditions, a characteristic of a nonlinear system.

Worksheet 2.12 This worksheet illustrates the possibility of using `DEplot` to produce the direction field and a set of trajectories in the phase space (when initial conditions are provided) in an integrated command, instead of using the combination of `odeplot` and `dfieldplot` as in the preceding worksheet; see `?DEtools,DEplot` for additional information.

```
> with(DEtools):
> mu := 1;
```

$$\mu := 1$$

```
> Eq0 := diff(x(t),t$2) + mu*(1 - x(t)^2)*diff(x(t),t) + x(t)=0;
```

$$Eq0 := (\tfrac{d^2}{dt^2}\,\mathrm{x}(t)) + (1 - \mathrm{x}(t)^2)\,(\tfrac{d}{dt}\,\mathrm{x}(t)) + \mathrm{x}(t) = 0$$

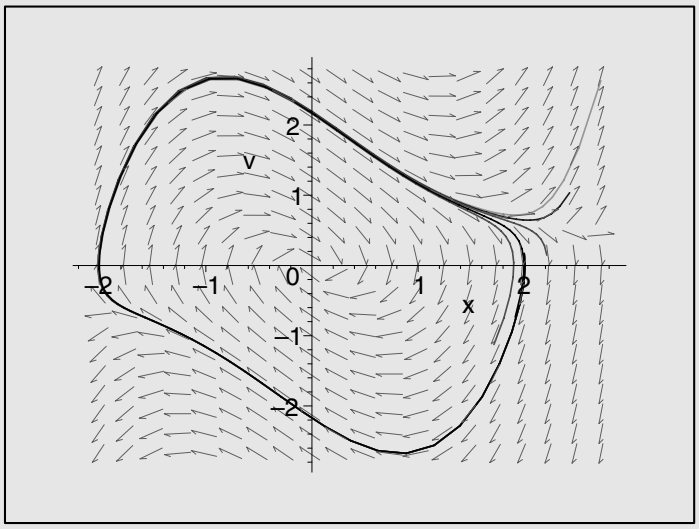
```
> Eq1 := diff(x(t),t) = v(t);
```

$$Eq1 := \tfrac{d}{dt}\,\mathrm{x}(t) = \mathrm{v}(t)$$

```
> Eq2 := subs(Eq1, Eq0);
```

$$Eq2 := (\tfrac{d}{dt}\,\mathrm{v}(t)) + (1 - \mathrm{x}(t)^2)\,\mathrm{v}(t) + \mathrm{x}(t) = 0$$

```
> DEplot([Eq1, Eq2], [x(t), v(t)], t=0..2.2*Pi, [[x(0)=2,
v(0)=0.169],
> [x(0)=2, v(0)=0.168], [x(0)=2, v(0)=0.170], [x(0)=2,
v(0)=0.1705],
> [x(0)=2, v(0)=0.171]], stepsize=0.1, linecolor=[black, red, red,
blue, green]);
```



Scientists traditionally work in a domain for which stable solutions exist, such as with a small angle for the pendulum system. A computer can evidently be of great assistance in helping scientists to explore a region of instability. In recent decades there has been much research in this area, and numerous books are published on this topic. Our purpose in this section is to introduce the representation of a dynamic system in the phase space, and bring an awareness of the tremendous utility of Maple in nonlinear dynamics. In Section 4.5 we will focus on the Duffing equation to study chaotic phenomena.

Exercises

1. For a system of forced oscillation, suppose that there is no damping; the differential equation governing such a system is

$$m\ddot{x} + kx = F_0 \cos(\omega t). \tag{2.25}$$

   Find the general solution to this equation.

2. Consider a numerical example for the above system:

$$\ddot{x} + x = 0.5\cos(0.8t), \quad x(0) = 0, \quad \dot{x}(0) = 0.$$

   Find the solution for x. Plot x as a function of time, and observe the modulation of the amplitude.

3. For a system with forced oscillation but without damping, if the driving frequency is equal to the natural frequency, such as for this equation,

$$\ddot{x} + x = 0.5 \cos t, \quad x(0) = 0, \quad \dot{x}(0) = 0,$$

find the solution for x and make a plot.

4. According to a model by Thomson, when a free electron of charge $-e$ and mass m is driven by a monochromatic electromagnetic wave, the electron is accelerated and so emits radiation. To fully understand this classical theory of scattering requires advanced knowledge of electromagnetism, but we offer this challenging problem for a reader to practice algebraic manipulation with Maple.

   (a) Motion of an electron is governed by this differential equation:

$$m\ddot{x} = -eE_0 \cos(\omega t). \tag{2.26}$$

   Show that the steady-state solution is

$$x = \frac{eE_0}{m\omega^2} \cos(\omega t) \equiv x_0 \cos(\omega t). \tag{2.27}$$

   (b) The power of radiation emitted by an accelerated electron is given in Chapter 10 in equation (10.75),

$$\overline{P} = \frac{e^2 x_0^2 \omega^4}{12\pi\epsilon_0 c^3}; \tag{2.28}$$

   identify x_0 from equation (2.27), so as to find $\overline{P}$.

   (c) The cross-section is defined as

$$\sigma = \frac{\overline{P}}{\overline{I}}, \tag{2.29}$$

   where the intensity of the incident wave is

$$\overline{I} = \frac{1}{2}\epsilon_0 c E_0^2. \tag{2.30}$$

   Show that

$$\sigma = \frac{1}{6} \frac{e^4}{\pi\epsilon_0^2 m^2 c^4}. \tag{2.31}$$

   This quantity is the Thomson cross-section.

   (d) The Thomson cross-section is commonly written as

$$\sigma = \frac{8\pi}{3} r_e^2, \tag{2.32}$$

where

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2} \tag{2.33}$$

is called the classical radius of an electron. Use Table A.1 to evaluate numerically both σ and r_e.
Hint: one might employ the `ScientificConstants` package (Maple 8 or higher) for physical constants.

5. Plot the direction field for

$$\ddot{x} + 0.125\dot{x} + x = 0;$$

this is the equation for damped oscillation in Section 2.2.2. Overlay the trajectory of the solution for an initial condition $x(0) = 2$ and $\dot{x}(0) = 0$.

6. For positive x and y, the system

$$\frac{dx}{dt} = x(1 - 0.5y), \tag{2.34a}$$
$$\frac{dy}{dt} = y(-0.75 + 0.25x) \tag{2.34b}$$

represents typical predator–prey equations,[2] a model encountered in mathematical biology. Plot the direction field for this system. Choose an initial condition such as $x(0) = 0.5$ and $y(0) = 2.0$ to find the numerical solution, and overlay the trajectory on the direction field. Make another plot showing two curves $x(t)$ versus t and $y(t)$ versus t.

7. For a hypothesized sequence of reactions involving reactants A and B, intermediates X and Y, and products D and E,

$$\begin{aligned} \mathrm{A} &\xrightarrow{k_1} \mathrm{X}, \\ \mathrm{B} + \mathrm{X} &\xrightarrow{k_2} \mathrm{Y} + \mathrm{D}, \\ 2\,\mathrm{X} + \mathrm{Y} &\xrightarrow{k_3} 3\,\mathrm{X}, \\ \mathrm{X} &\xrightarrow{k_4} \mathrm{E}, \end{aligned}$$

the concentrations of X and Y exhibit oscillatory behavior during the reaction. According to chemical kinetics, X and Y are governed by the so-called *Brusselator* equations:[3]

$$\frac{d\,\mathrm{X}}{dt} = k_1\,\mathrm{A} - k_2\,\mathrm{B}\,\mathrm{X} + k_3\,\mathrm{X}^2\,\mathrm{Y} - k_4\,\mathrm{X}, \tag{2.35a}$$
$$\frac{d\,\mathrm{Y}}{dt} = k_2\,\mathrm{B}\,\mathrm{X} - k_3\,\mathrm{X}^2\,\mathrm{Y}. \tag{2.35b}$$

[2] Boyce and Diprima 2001, § 9.5, p. 503.

[3] I. Prigogine and R. Lefever, "Symmetry breaking instabilities in dissipative systems," *Journal of Chemical Physics*, **48**, 1695–1700 (1968); D. Kondepudi and I. Prigogine, *Modern Thermodynamics*, Chichester; New York: Wiley, 1998, p. 438ff.

We assume that $k_1 = 1.0$, $k_2 = 1.0$, $k_3 = 1.0$, $k_4 = 1.0$, A $= 1.0$, B $= 3.0$, and X and Y are functions of time t. For $\mathrm{X}(0) = 1.0$ and $\mathrm{Y}(0) = 1.0$, find the numerical solution; plot $\mathrm{X}(t)$ versus t and $\mathrm{Y}(t)$ versus t. In another plot overlay the trajectory in the phase space on the direction field. They should resemble Figure 2.2.

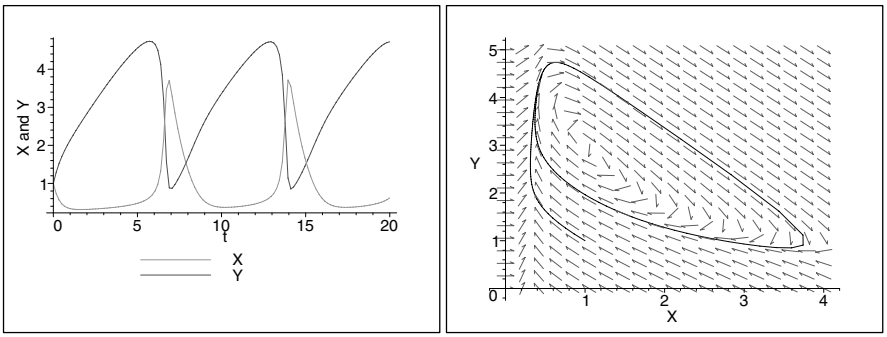


Figure 2.2: Solution to equation (2.35).

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3 Calculus of Variations

The calculus of variations involves minimizing expressions that depend on a function. The objective is not merely to discover a point at which some particular function assumes a minimum value, but to determine an entire dependence of some function in such a way that it minimizes an integral involving that function and its derivatives. This problem played an important role in classical physics during the eighteenth and nineteenth centuries, and in quantum mechanics and relativity during the twentieth century. For these applications, Maple proves useful particularly in the following ways: to obtain the Lagrangian requires a coordinate transformation; in formulating equations of motion, calculus involving the chain rule is generally tedious. In this chapter we develop a method with Maple that we can apply systematically to diminish the extent of manual manipulation.

3.1 Euler–Lagrange Equation

We first consider a problem in one-dimensional form. A function $f(y, y', x)$ is defined on a path $y = y(x)$ between two values x_A and x_B, where y' is the derivative of y with respect to x,

$$y' \equiv \frac{dy}{dx}. \tag{3.1}$$

We seek a particular path $y(x)$ such that the line integral J,

$$J = \int_{x_A}^{x_B} f(y, y', x)dx, \tag{3.2}$$

has an extremal value. We consider x to be the independent variable, and y and y' two separate dependent variables. The solution of this problem requires that the following condition be satisfied:

$$\boxed{\frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right) - \frac{\partial f}{\partial y} = 0}. \tag{3.3}$$

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ISBN: 3-527-40640-9

The derivation can be found in many books,[1] which justifies our omission. Equation (3.3), called the Euler–Lagrange equation, is a most useful equation that recurs many times in this book.

3.2 Mathematical Examples

There are several famous problems of the calculus of variations. To demonstrate how to use the Euler–Lagrange equation in Maple, we begin with a simple problem: what is the plane curve connecting two given points having the shortest length?

The line element in a plane is the infinitesimal separation between two points:

$$ds = \sqrt{dx^2 + dy^2}; \tag{3.4}$$

the total length of any curve between the points $\mathcal{A}$ and $\mathcal{B}$ is hence

$$J = \int_{\mathcal{A}}^{\mathcal{B}} ds = \int_{x_A}^{x_B} \sqrt{1 + \left(\frac{dy}{dx}\right)^2}\, dx. \tag{3.5}$$

We identify f as the integrand,

$$f = \sqrt{1 + y'^2}.$$

Substituting f into the Euler–Lagrange equation and solving the differential equation, we would obtain the desired function.

Maple contains a package `VariationalCalculus` that allows one to employ the Euler–Lagrange equation in an integrated procedure. Instead of using this package, we develop a method of solving this type of problem explicitly from the original equation. According to the Euler–Lagrange equation, one must differentiate a function $f(y, y', x)$ with respect to two related functions, $y(x)$ and $y'(x)$, but the `diff` command fails to support the performance of such a task without invoking an external library or inserting a procedure. Our approach is to treat $y(x)$ and $y'(x)$ as separate variables by substituting distinct symbolic quantities for them, so that Maple can differentiate with respect to those symbols. We then substitute back those symbols with their original assignments, and continue to calculate the second derivative with respect to the independent variable x, and solve the differential equations. We outline the method as follows.

- Define `f` as a function of `x`, `y(x)`, and `diff(y(x),x)`.
- Substitute `y(x)` and `diff(y(x),x)` by two symbols, for example `var1` and `var2` respectively, `f1 := subs({y(x)=var1, diff(y(x),x)=var2}, f);`, so that `f1` becomes a function of `var1` and `var2`.

[1] Goldstein et al. 2002, p. 36ff.

- Differentiate `f1` with respect to `var1` and `var2`: `Epr1 := diff(f1, var2);` `Epr2:=diff(f1, var1);`.
- Replace `var1` and `var2` with their original assignments in `Epr1` and `Epr2`:
  `Epr3 := subs({var1=y(x), var2=diff(y(x),x)}, Epr1);`
  `Epr4 := subs({var1=y(x), var2=diff(y(x),x)}, Epr2);`.
- Differentiate `Epr3` with respect to `x`: `Epr5 := diff(Epr3,x);`
- The Euler–Lagrange equation states that `Eq6 := Epr5 - Epr4 = 0;`.
- Use the `dsolve` command to solve the differential equation.

These substitutions might appear tedious, but they are readily accomplished with routine editing operations such as "cut" and "paste." We consider that they enable a direct approach to the solution of each problem step by step, and we oversee each operation.

Worksheet 3.1 In this worksheet, we define a function `f`, then substitute y with `var1` and y' with `var2`, according to the method outlined above.

```
> f := sqrt(1 + diff(y(x),x)^2);
```

$$f := \sqrt{1 + (\tfrac{d}{dx}\,\mathrm{y}(x))^2}$$

```
> f1 := subs({y(x)=var1, diff(y(x),x)=var2}, f);
```

$$f1 := \sqrt{1 + var2^2}$$

```
> Epr1 := diff(f1, var2);
```

$$Epr1 := \frac{var2}{\sqrt{1 + var2^2}}$$

```
> Epr2 := diff(f1, var1);
```

$$Epr2 := 0$$

```
> Epr3 := subs({var1=y(x), var2=diff(y(x),x)}, Epr1);
```

$$Epr3 := \frac{\frac{d}{dx}\,\mathrm{y}(x)}{\sqrt{1 + (\frac{d}{dx}\,\mathrm{y}(x))^2}}$$

```
> Epr4 := subs({var1=y(x), var2=diff(y(x),x)}, Epr2);
```

$$Epr4 := 0$$

```
> Epr5 := diff(Epr3, x);
```

$$Epr5 := -\frac{(\frac{d}{dx}\,\mathrm{y}(x))^2\,(\frac{d^2}{dx^2}\,\mathrm{y}(x))}{(1 + (\frac{d}{dx}\,\mathrm{y}(x))^2)^{(3/2)}} + \frac{\frac{d^2}{dx^2}\,\mathrm{y}(x)}{\sqrt{1 + (\frac{d}{dx}\,\mathrm{y}(x))^2}}$$

```
> Eq6 := Epr5 - Epr4 = 0;
```

$$Eq6 := -\frac{(\frac{d}{dx}\,\mathrm{y}(x))^2\,(\frac{d^2}{dx^2}\,\mathrm{y}(x))}{(1+(\frac{d}{dx}\,\mathrm{y}(x))^2)^{(3/2)}} + \frac{\frac{d^2}{dx^2}\,\mathrm{y}(x)}{\sqrt{1+(\frac{d}{dx}\,\mathrm{y}(x))^2}} = 0$$

```
> Soln1 := dsolve(Eq6, y(x));
```

$$Soln1 := \mathrm{y}(x) = _C1\,x + _C2$$

We obtain the solution for the shortest distance between two points; as expected, it is a straight line,

$$y = c_1 x + c_2. \tag{3.6}$$

Example 3.1 The brachistochrone problem is the following: given two points $\mathcal{A}$ and $\mathcal{B}$ in a vertical plane, characterize a curve joining two points along which a particle falling from rest under the influence of gravity travels from the higher to the lower point in the least amount of time.

Solution Let v be the speed of the particle along the curve; the required time of transit is

$$t = \int_{\mathcal{A}}^{\mathcal{B}} \frac{ds}{v}. \tag{3.7}$$

From the conservation of energy, we find v:

$$\frac{1}{2}mv^2 = mgy, \quad v = \sqrt{2gy}. \tag{3.8}$$

With the line element ds the same as in the preceding problem, we have an integral

$$t = \int_{x_A}^{x_B} \sqrt{\frac{1+y'^2}{2gy}}\,dx. \tag{3.9}$$

Defining the integrand as f,

$$f = \sqrt{\frac{1+y'^2}{y}},$$

and employing the technique described above, we find the condition for the minimum time. Upon use of the `dsolve` command, Maple delivers an implicit solution, which relates y to x as

$$\sqrt{-y^2+c_1 y} - \frac{c_1}{2}\tan^{-1}\frac{y-\frac{c_1}{2}}{\sqrt{-y^2+c_1 y}} - x - c_2 = 0. \tag{3.10}$$

Worksheet 3.2 The substitutions are the same as in the preceding worksheet.

```
> f := sqrt((1 + diff(y(x),x)^2)/y(x));
```

$$f := \sqrt{\frac{1 + (\frac{d}{dx}\,\mathrm{y}(x))^2}{\mathrm{y}(x)}}$$

```
> f1 := subs({y(x)=var1, diff(y(x),x)=var2}, f);
```

$$f1 := \sqrt{\frac{1 + var2^2}{var1}}$$

```
> Epr1 := diff(f1, var2);
```

$$Epr1 := \frac{var2}{\sqrt{\frac{1 + var2^2}{var1}}\, var1}$$

```
> Epr2 := diff(f1, var1);
```

$$Epr2 := -\frac{1 + var2^2}{2\sqrt{\frac{1 + var2^2}{var1}}\, var1^2}$$

```
> Epr3 := subs({var1=y(x), var2=diff(y(x),x)}, Epr1);
```

$$Epr3 := \frac{\frac{d}{dx}\,\mathrm{y}(x)}{\sqrt{\frac{1 + (\frac{d}{dx}\,\mathrm{y}(x))^2}{\mathrm{y}(x)}}\,\mathrm{y}(x)}$$

```
> Epr4 := subs({var1=y(x), var2=diff(y(x),x)}, Epr2);
```

$$Epr4 := -\frac{1}{2}\,\frac{1 + (\frac{d}{dx}\,\mathrm{y}(x))^2}{\sqrt{\frac{1 + (\frac{d}{dx}\,\mathrm{y}(x))^2}{\mathrm{y}(x)}}\,\mathrm{y}(x)^2}$$

```
> Epr5 := diff(Epr3, x);
```

$$Epr5 := -\frac{1}{2}\,\frac{(\frac{d}{dx}\,\mathrm{y}(x))\left(\frac{2\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^2}{dx^2}\,\mathrm{y}(x))}{\mathrm{y}(x)} - \frac{\%1\,(\frac{d}{dx}\,\mathrm{y}(x))}{\mathrm{y}(x)^2}\right)}{\left(\frac{\%1}{\mathrm{y}(x)}\right)^{(3/2)}\,\mathrm{y}(x)} + \frac{\frac{d^2}{dx^2}\,\mathrm{y}(x)}{\sqrt{\frac{\%1}{\mathrm{y}(x)}}\,\mathrm{y}(x)} - \frac{(\frac{d}{dx}\,\mathrm{y}(x))^2}{\sqrt{\frac{\%1}{\mathrm{y}(x)}}\,\mathrm{y}(x)^2}$$

$$\%1 := 1 + (\tfrac{d}{dx}\,\mathrm{y}(x))^2$$

```
> Eq6 := Epr5 - Epr4 = 0;
```

$$Eq6 := -\frac{1}{2}\frac{(\frac{d}{dx}\,\mathrm{y}(x))\left(\dfrac{2\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^2}{dx^2}\,\mathrm{y}(x))}{\mathrm{y}(x)} - \dfrac{\%1\,(\frac{d}{dx}\,\mathrm{y}(x))}{\mathrm{y}(x)^2}\right)}{\left(\dfrac{\%1}{\mathrm{y}(x)}\right)^{(3/2)}\mathrm{y}(x)} + \frac{\frac{d^2}{dx^2}\,\mathrm{y}(x)}{\sqrt{\dfrac{\%1}{\mathrm{y}(x)}}\,\mathrm{y}(x)} - \frac{(\frac{d}{dx}\,\mathrm{y}(x))^2}{\sqrt{\dfrac{\%1}{\mathrm{y}(x)}}\,\mathrm{y}(x)^2} + \frac{1}{2}\frac{\%1}{\sqrt{\dfrac{\%1}{\mathrm{y}(x)}}\,\mathrm{y}(x)^2} = 0$$

$$\%1 := 1 + (\tfrac{d}{dx}\,\mathrm{y}(x))^2$$

```
> Soln1 := dsolve(Eq6, y(x));
```

$$Soln1 := -\sqrt{\%1} + \frac{1}{2}_C1\,\arctan\left(\frac{\mathrm{y}(x) - \frac{_C1}{2}}{\sqrt{\%1}}\right) - x - _C2 = 0,$$

$$\sqrt{\%1} - \frac{1}{2}_C1\,\arctan\left(\frac{\mathrm{y}(x) - \frac{_C1}{2}}{\sqrt{\%1}}\right) - x - _C2 = 0$$

$$\%1 := -\mathrm{y}(x)^2 + _C1\,\mathrm{y}(x)$$

To express the result in a parametric form, we make some manual rearrangements. Introducing a parameter η defined as

$$\tan\eta = \frac{y - \frac{c_1}{2}}{\sqrt{-y^2 + c_1 y}}, \tag{3.11}$$

and after some trigonometric arrangement we find that

$$\sqrt{-y^2 + c_1 y} = \frac{c_1}{2}\cos\eta. \tag{3.12}$$

We write equation (3.10) as

$$x = \frac{c_1}{2}(\cos\eta - \eta) - c_2, \tag{3.13a}$$

$$y = \frac{c_1}{2}(\sin\eta + 1). \tag{3.13b}$$

These equations generate a cycloid, which represents the motion of a fixed point on the circumference of a circle of radius $c_1/2$ that rolls on the line $y = 0$. We plot the curve below.

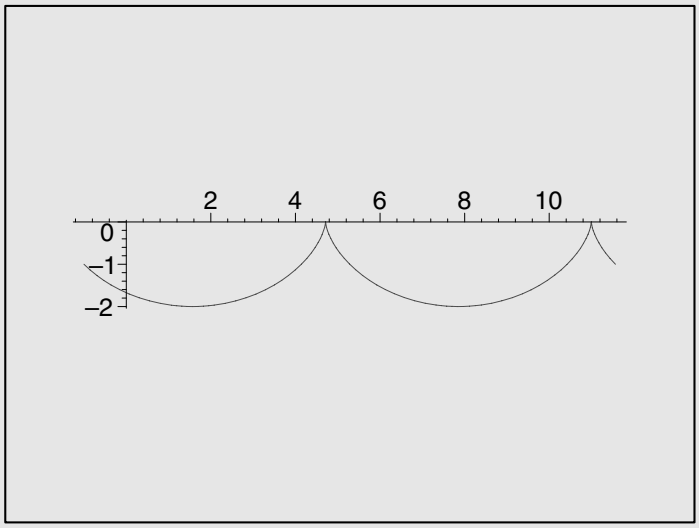
Worksheet 3.3 We demonstrate an example of the `plot` command for functions in parametric form. The coefficients are set to be $c_1 = -2$ and $c_2 = 0$. To produce a parametric plot,

we place the x and y expressions with the name (in this example η) and range (0 to 4π) of the parameter in a list (thus enclosed within brackets).

```
> c1 := -2; c2 := 0;
```

$$c1 := -2$$
$$c2 := 0$$

```
> plot([c1/2*(cos(eta) - eta) - c2, c1/2*(sin(eta) + 1),
> eta=0..4*Pi], scaling=constrained);
```



Example 3.2 Find the geodesic, which is a curve that corresponds to an extremum of the distance between two points on the surface of a sphere.

Solution On a sphere of fixed radius a, the line element is

$$ds^2 = a^2 d\theta^2 + a^2 \sin^2\theta \, d\phi^2. \tag{3.14}$$

We make a transformation $x \to \phi$, $y \to \theta$ in the above formulation, so that ϕ becomes the independent variable and θ is the dependent one that is hence a function of ϕ. The length of the curve is

$$J = \int ds = \int \sqrt{a^2 \left(\frac{d\theta}{d\phi}\right)^2 + a^2 \sin^2\theta} \, d\phi. \tag{3.15}$$

We identify f as

$$f = \sqrt{a^2 \left(\frac{d\theta}{d\phi}\right)^2 + a^2 \sin^2\theta}.$$

Applying the Euler–Lagrange equation, and solving the differential equation, we obtain a solution

$$\theta = -\tan^{-1}\left(\frac{1}{2}\frac{1}{c_1\sin\phi - c_2\cos\phi}\right). \tag{3.16}$$

Worksheet 3.4 The substitutions are similar to those in preceding examples: θ and $\frac{d\theta}{d\phi}$ are assigned to be `var1` and `var2` respectively.

```
> f := sqrt(a^2*diff(theta(phi),phi)^2 + a^2*sin(theta(phi))^2);
```

$$f := \sqrt{a^2\,(\tfrac{d}{d\phi}\,\theta(\phi))^2 + a^2\sin(\theta(\phi))^2}$$

```
> f1:=subs({theta(phi)=var1, diff(theta(phi),phi)=var2}, f);
```

$$f1 := \sqrt{a^2\ var2^2 + a^2\sin(var1)^2}$$

```
> Epr1 := diff(f1, var2);
```

$$Epr1 := \frac{a^2\ var2}{\sqrt{a^2\ var2^2 + a^2\sin(var1)^2}}$$

```
> Epr2 := diff(f1, var1);
```

$$Epr2 := \frac{a^2\sin(var1)\cos(var1)}{\sqrt{a^2\ var2^2 + a^2\sin(var1)^2}}$$

```
> Epr3 := subs({var1=theta(phi), var2=diff(theta(phi),phi)},
> Epr1);
```

$$Epr3 := \frac{a^2\,(\tfrac{d}{d\phi}\,\theta(\phi))}{\sqrt{a^2\,(\tfrac{d}{d\phi}\,\theta(\phi))^2 + a^2\sin(\theta(\phi))^2}}$$

```
> Epr4 := subs({var1=theta(phi), var2=diff(theta(phi),phi)},
> Epr2);
```

$$Epr4 := \frac{a^2\sin(\theta(\phi))\cos(\theta(\phi))}{\sqrt{a^2\,(\tfrac{d}{d\phi}\,\theta(\phi))^2 + a^2\sin(\theta(\phi))^2}}$$

```
> Epr5 := diff(Epr3, phi);
```

$$Epr5 := -\frac{1}{2}\,\frac{a^2\,\%1\,(2\,a^2\,\%1\,(\tfrac{d^2}{d\phi^2}\,\theta(\phi)) + 2\,a^2\sin(\theta(\phi))\cos(\theta(\phi))\,\%1)}{(a^2\,\%1^2 + a^2\sin(\theta(\phi))^2)^{(3/2)}}$$
$$+ \frac{a^2\,(\tfrac{d^2}{d\phi^2}\,\theta(\phi))}{\sqrt{a^2\,\%1^2 + a^2\sin(\theta(\phi))^2}}$$
$$\%1 := \tfrac{d}{d\phi}\,\theta(\phi)$$

```
> Eq6 := Epr5 - Epr4 = 0;
```

$$Eq6 := -\frac{1}{2}\frac{a^2\,\%1\,(2\,a^2\,\%1\,(\frac{d^2}{d\phi^2}\,\theta(\phi)) + 2\,a^2\sin(\theta(\phi))\cos(\theta(\phi))\,\%1)}{\%2^{(3/2)}} + \frac{a^2\,(\frac{d^2}{d\phi^2}\,\theta(\phi))}{\sqrt{\%2}}$$
$$- \frac{a^2\sin(\theta(\phi))\cos(\theta(\phi))}{\sqrt{\%2}} = 0$$
$$\%1 := \frac{d}{d\phi}\,\theta(\phi)$$
$$\%2 := a^2\,\%1^2 + a^2\sin(\theta(\phi))^2$$

```
> Eq7 := simplify(Eq6);
```

$$Eq7 := -a^2(2\,(\frac{d}{d\phi}\,\theta(\phi))^2\sin(\theta(\phi))\cos(\theta(\phi)) - (\frac{d^2}{d\phi^2}\,\theta(\phi)) + (\frac{d^2}{d\phi^2}\,\theta(\phi))\cos(\theta(\phi))^2$$
$$+ \sin(\theta(\phi))\cos(\theta(\phi)) - \sin(\theta(\phi))\cos(\theta(\phi))^3)\Big/(((\frac{d}{d\phi}\,\theta(\phi))^2 + 1 - \cos(\theta(\phi))^2)$$
$$\sqrt{a^2\,((\frac{d}{d\phi}\,\theta(\phi))^2 + 1 - \cos(\theta(\phi))^2)}) = 0$$

```
> Soln1 := dsolve(Eq7, theta(phi));
```

$$Soln1 := \theta(\phi) = \arctan\left(\frac{1}{2}\,\frac{1}{-\sin(\phi)\,_C1 + _C2\cos(\phi)}\right)$$

We verify the solution by transforming to Cartesian coordinates. With a substitution

$$\phi = \tan^{-1}\frac{y}{x}, \tag{3.17a}$$

$$\theta = \cos^{-1}\frac{z}{\sqrt{x^2+y^2+z^2}}, \tag{3.17b}$$

Maple gives

$$z = -2c_2x + 2c_2y, \tag{3.18}$$

which represents a plane that passes the origin at the center of the sphere. The intersection of this plane with the sphere $r = a$ produces a geodesic, or a great circle, on the surface of the sphere.

Worksheet 3.5 The transformation of coordinates involves a simple command `subs`. We use the `isolate` command, to isolate z on the left side of the equation.

```
> Eq11 := theta = -arctan(1/2*1/(_C1*sin(phi) - _C2*cos(phi))):
> Eq12 := subs({theta=arccos(z/sqrt(x^2 + y^2 + z^2)),
> phi=arctan(y/x)}, Eq11):
> Eq13 := simplify(Eq12):
> Eq14 := isolate(Eq13, z);
```

$$Eq14 := z = -2\,_C1\,y + 2\,_C2\,x$$

3.3 Symmetry Properties

Symmetry plays a fundamental role in physics, and we often exploit this subject in classical mechanics. We use a mathematical example to demonstrate one type of symmetry – translational invariance. Suppose that a function $f(y, y', x)$ contains no explicit appearance of y, although it may contain y', then

$$\frac{\partial f}{\partial y} = 0;$$

the Euler–Lagrange equation becomes

$$\frac{d}{dx}\frac{\partial f}{\partial y'} = 0;$$

hence

$$\frac{\partial f}{\partial y'} = \text{constant}. \tag{3.19}$$

The order of the differential equation is reduced from second to first.

Example 3.3 Find the surface of revolution about the y axis with minimum area that passes two given fixed points, (x_A, y_A) and (x_B, y_B).

Solution We seek to minimize the surface area,

$$J = \int_{\mathcal{A}}^{\mathcal{B}} 2\pi x \, ds = 2\pi \int_{x_A}^{x_B} x\sqrt{1 + y'^2}\, dx. \tag{3.20}$$

Defining f as

$$f = x\sqrt{1 + y'^2},$$

we notice that f contains no explicit dependence on y. This situation reflects the fact that there is no preferred origin for y: a transformation $y \to y + \epsilon$, namely an arbitrary shift of the origin, does not alter the result. Therefore, we need only to solve

$$\frac{\partial f}{\partial y'} = a, \tag{3.21}$$

where a is a constant.

Worksheet 3.6 The substitutions are similar to those in preceding worksheets; we assign a constant `a` as discussed above.

```
> f := x*sqrt(1 + (diff(y(x),x))^2);
```

$$f := x\sqrt{1+(\tfrac{d}{dx}\,\mathrm{y}(x))^2}$$

```
> f1 := subs({y(x)=var1, diff(y(x),x)=var2}, f);
```

$$f1 := x\sqrt{1+var2^2}$$

```
> Epr1 := diff(f1, var2);
```

$$Epr1 := \frac{x\,var2}{\sqrt{1+var2^2}}$$

```
> Epr2 := diff(f1, var1);
```

$$Epr2 := 0$$

```
> Epr3 := subs({var1=y(x), var2=diff(y(x),x)}, Epr1);
```

$$Epr3 := \frac{x\,(\frac{d}{dx}\,\mathrm{y}(x))}{\sqrt{1+(\frac{d}{dx}\,\mathrm{y}(x))^2}}$$

```
> Eq6 := Epr3 = a;
```

$$Eq6 := \frac{x\,(\frac{d}{dx}\,\mathrm{y}(x))}{\sqrt{1+(\frac{d}{dx}\,\mathrm{y}(x))^2}} = a$$

```
> Soln1 := dsolve(Eq6, y(x));
```

$$Soln1 := \mathrm{y}(x) = a\ln(x+\sqrt{x^2-a^2})+_C1,\ \mathrm{y}(x) = -a\ln(x+\sqrt{x^2-a^2})+_C1$$

Using Maple we obtain

$$y = a\ln(x+\sqrt{x^2-a^2})+c_1. \tag{3.22}$$

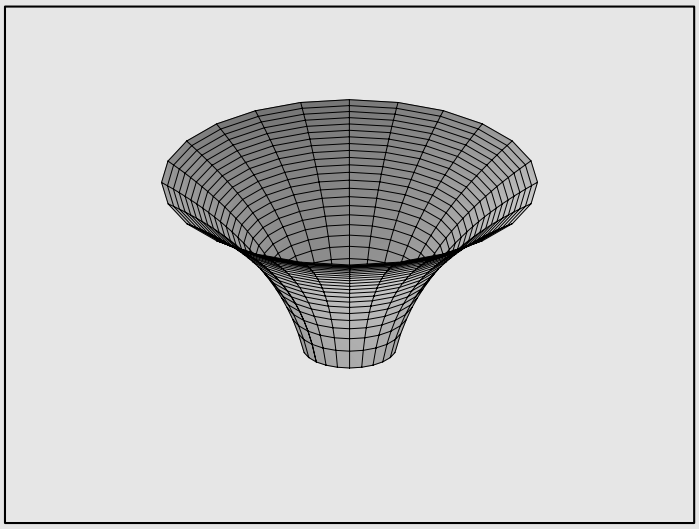
This curve is called a catenary; we plot the surface of revolution in the next worksheet.

Worksheet 3.7 In this example, we demonstrate the method of plotting a surface of revolution around the z axis using the `plot3d` command in parametric form. We provide a list containing the x, y and z expressions, and the name and range of two parameters (in this example ρ and ϕ). The x expression is $\rho\cos\phi$, and the y expression is $\rho\sin\phi$, with the range of ϕ from 0 to 2π.

```
> z := ln(rho + sqrt(rho^2 - 1));
```

$$z := \ln(\rho+\sqrt{\rho^2-1})$$

```
> plot3d([rho*cos(phi), rho*sin(phi), z], rho=1.2..4.8,
> phi=0..2*Pi);
```



3.4 Principle of Least Action

Newton's second law expressed as $F = ma$ is a differential equation because a is the second derivative of the coordinate with respect to time, yet classical mechanics has an alternative formulation in an integral form. *Hamilton's principle* states that the motion of a particle from time t_1 to t_2 is such that the time integral

$$S = \int_{t_1}^{t_2} L\,dt \tag{3.23}$$

takes the least value for the correct path of motion. The quantity S is called the *action*, and the integrand L is called the *Lagrangian*.

In classical mechanics, the Lagrangian for a particle of mass m moving in an arbitrary potential field is the difference between the kinetic energy and potential energy,

$$L(q, \dot{q}, t) = T - V = \frac{m\dot{q}^2}{2} - V(q). \tag{3.24}$$

A Lagrangian in its most general form is a function of a coordinate q, its derivative $\dot{q}$, and time t; the reason that we write q, which signifies the generalized coordinate, will be discussed in the next section. We apply the mathematical formalism of the calculus of variations to physics through these transformations:

$$x \to t,$$

$$y \to q,$$
$$y' \to \dot{q} \equiv \frac{dq}{dt},$$
$$f(y, y', t) \to L(q, \dot{q}, t).$$

Finding the equation of motion simply involves solving the differential equation derived from the Euler–Lagrange equation,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0. \tag{3.25}$$

Applying this equation to the Lagrangian of one particle, we obtain

$$m\ddot{q} + \frac{\partial V}{\partial q} = 0; \tag{3.26}$$

because $-\partial V/\partial q$ is the force, the Lagrangian formalism reproduces Newton's second law in the familiar form,

$$F = ma. \tag{3.27}$$

One advantage of mechanics in a Lagrangian formulation is that in some situations the force diagram is complicated, but one can readily identify energy. We provide the following example to demonstrate this concept.

Example 3.4 A particle of mass m_2 slides without friction along a wedge of angle α and mass m_1 that can move without friction on a horizontal surface. Find the acceleration of the wedge.

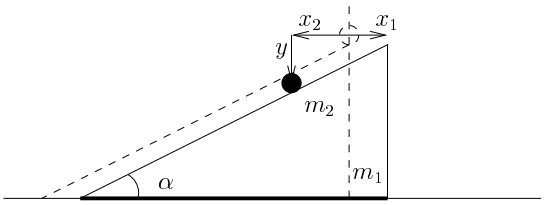


Figure 3.1: A particle of mass m_2 sliding along a wedge of mass m_1 on a smooth surface.

Solution The coordinates are defined in Figure 3.1; the origin is set on the top of the wedge at $t = 0$. The kinetic energy of the system is

$$T = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_2\dot{y}^2,$$

and the potential energy is

$$V = m_2 g y.$$

From the conservation of momentum, the horizontal component of the center of mass remains fixed; we have

$$m_1 x_1 + m_2 x_2 = 0, \quad x_2 = -\frac{m_1}{m_2} x_1.$$

Because the block m_2 is restricted to move along the wedge, we have

$$\frac{y}{x_2 - x_1} = \tan\alpha.$$

With these two equations, we can write x_2 and y in terms of x_1, so as to express the Lagrangian with only one dependent variable. We define $x_1 = q(t)$, and obtain L as a function of $q(t)$ and $\dot{q}(t)$. These substitutions (using Maple) yield the Lagrangian as

$$\begin{aligned} L = {} & \frac{1}{2} m_1 \left(1 + \frac{m_1}{m_2}\right) \dot{q}^2 + \frac{1}{2} m_2 \tan^2\alpha \left(1 + \frac{m_1}{m_2}\right)^2 \dot{q}^2 \\ & + m_2 g \tan\alpha \left(1 + \frac{m_1}{m_2}\right) q. \end{aligned} \tag{3.28}$$

Substituting L into the Euler–Lagrange equation, we obtain the equation of motion:

$$m_1 \left(1 + \frac{m_1}{m_2}\right) \ddot{q} + m_2 \tan^2\alpha \left(1 + \frac{m_1}{m_2}\right)^2 \ddot{q} - m_2 g \tan\alpha \left(1 + \frac{m_1}{m_2}\right) = 0.$$

After we isolate $\ddot{q}$ from the differential equation, the acceleration of the wedge is identified as

$$a = \ddot{q} = \frac{m_2\, g\, \tan\alpha}{m_1 + (m_1 + m_2)\tan^2\alpha}.$$

Worksheet 3.8 We assign `x1`, `x2` and `y`, as defined above, and have Maple rearrange expressions for kinetic and potential energies. Our derivation of an equation of motion involves the same technique as we have employed in preceding worksheets. We use the `isolate` command to isolate an expression on the left-hand side of the equation.

```
> x1 := q(t);
```

$$x1 := \mathrm{q}(t)$$

```
> x2 := -m1/m2*x1;
```

$$x2 := -\frac{m1\ \mathrm{q}(t)}{m2}$$

```
> y := (x2-x1)*tan(alpha);
```

$$y := \left(-\frac{m1\ \mathrm{q}(t)}{m2} - \mathrm{q}(t)\right) \tan(\alpha)$$

```
> T := 1/2*m1*diff(x1,t)^2 + 1/2*m2*diff(x2,t)^2 +
> 1/2*m2*diff(y,t)^2;
```

$$T := \frac{1}{2} m1\,(\tfrac{d}{dt}\,\mathrm{q}(t))^2 + \frac{1}{2}\frac{m1^2\,(\frac{d}{dt}\,\mathrm{q}(t))^2}{m2} + \frac{1}{2} m2 \left(-\frac{m1\,(\frac{d}{dt}\,\mathrm{q}(t))}{m2} - (\tfrac{d}{dt}\,\mathrm{q}(t))\right)^2 \tan(\alpha)^2$$

```
> V := m2*g*y;
```

$$V := m2\,g \left(-\frac{m1\,\mathrm{q}(t)}{m2} - \mathrm{q}(t)\right) \tan(\alpha)$$

```
> L := T-V;
```

$$L := \frac{1}{2} m1\,(\tfrac{d}{dt}\,\mathrm{q}(t))^2 + \frac{1}{2}\frac{m1^2\,(\frac{d}{dt}\,\mathrm{q}(t))^2}{m2} + \frac{1}{2}\,m2 \left(-\frac{m1\,(\frac{d}{dt}\,\mathrm{q}(t))}{m2} - (\tfrac{d}{dt}\,\mathrm{q}(t))\right)^2 \tan(\alpha)^2$$
$$-m2\,g \left(-\frac{m1\,\mathrm{q}(t)}{m2} - \mathrm{q}(t)\right) \tan(\alpha)$$

```
> L1 := subs({q(t)=var1, diff(q(t),t)=var2}, L);
```

$$L1 := \frac{m1\ var2^2}{2} + \frac{m1^2\ var2^2}{2\,m2} + \frac{1}{2}\,m2 \left(-\frac{m1\ var2}{m2} - var2\right)^2 \tan(\alpha)^2$$
$$- m2\,g \left(-\frac{m1\ var1}{m2} - var1\right) \tan(\alpha)$$

```
> Epr1 := diff(L1, var2);
```

$$Epr1 := m1\ var2 + \frac{m1^2\ var2}{m2} + m2 \left(-\frac{m1\ var2}{m2} - var2\right) \tan(\alpha)^2 \left(-\frac{m1}{m2} - 1\right)$$

```
> Epr2 := diff(L1, var1);
```

$$Epr2 := -m2\,g \left(-\frac{m1}{m2} - 1\right) \tan(\alpha)$$

```
> Epr3 := subs({var1=q(t), var2=diff(q(t),t)}, Epr1);
```

$$Epr3 := m1\,(\tfrac{d}{dt}\,\mathrm{q}(t)) + \frac{m1^2\,(\frac{d}{dt}\,\mathrm{q}(t))}{m2}$$
$$+m2 \left(-\frac{m1\,(\frac{d}{dt}\,\mathrm{q}(t))}{m2} - (\tfrac{d}{dt}\,\mathrm{q}(t))\right) \tan(\alpha)^2 \left(-\frac{m1}{m2} - 1\right)$$

```
> Epr4 := subs({var1=q(t), var2=diff(q(t),t)}, Epr2);
```

$$Epr4 := -m2\,g \left(-\frac{m1}{m2} - 1\right) \tan(\alpha)$$

```
> Epr5 := diff(Epr3, t);
```

$$Epr5 := m1\,(\tfrac{d^2}{dt^2}\,\mathrm{q}(t)) + \frac{m1^2\,(\frac{d^2}{dt^2}\,\mathrm{q}(t))}{m2}$$
$$+m2 \left(-\frac{m1\,(\frac{d^2}{dt^2}\,\mathrm{q}(t))}{m2} - (\tfrac{d^2}{dt^2}\,\mathrm{q}(t))\right) \tan(\alpha)^2 \left(-\frac{m1}{m2} - 1\right)$$

```
> Eq6 := Epr5 - Epr4 = 0;
```

$$Eq6 := m1\,(\tfrac{d^2}{dt^2}\,\mathrm{q}(t)) + \frac{m1^2\,(\frac{d^2}{dt^2}\,\mathrm{q}(t))}{m2} + m2\left(-\frac{m1\,(\frac{d^2}{dt^2}\,\mathrm{q}(t))}{m2} - (\tfrac{d^2}{dt^2}\,\mathrm{q}(t))\right)\tan(\alpha)^2\left(-\frac{m1}{m2} - 1\right) + m2\,g\left(-\frac{m1}{m2} - 1\right)\tan(\alpha) = 0$$

```
> Eq7 := simplify(isolate(Eq6, diff(q(t),t$2)));
```

$$Eq7 := \tfrac{d^2}{dt^2}\,\mathrm{q}(t) = \frac{m2\tan(\alpha)\,g}{m1 + m1\tan(\alpha)^2 + \tan(\alpha)^2\,m2}$$

3.5 Systems with Many Degrees of Freedom

To describe the position of a system of N particles in space, we generally need $3N$ coordinates. In some situations, particles' Cartesian coordinates are not independent of each other. The number of independent quantities which must be specified to define the position of a system is called the number of degrees of freedom. Any n quantities q_1, q_2, …, q_n which completely define the position of a system with n degrees of freedom are called generalized coordinates, which can be distances, angles, and so on. Generalized coordinates are related to Cartesian coordinates through the *transformation equations*. We demonstrate such transformations in an example below.

Suppose that L is a function of generalized coordinates q_1, q_2, …, q_n, and their derivatives with respect to time are $\dot{q_1}$, $\dot{q_2}$, …, $\dot{q_n}$,

$$L = L(q_1, q_2, \ldots, q_n, \dot{q}_1, \dot{q}_2, \ldots, \dot{q}_n, t), \tag{3.29}$$

the Euler–Lagrange equation becomes

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0, \quad i = 1, 2, \ldots, n. \tag{3.30}$$

The generalized momentum conjugate to a generalized coordinate q_i is

$$p_i \equiv \frac{\partial L}{\partial \dot{q}_i}. \tag{3.31}$$

If some particular generalized coordinate q_k is absent from a Lagrangian L (although $\dot{q}_k$ might not be), we call it an *ignorable* coordinate. According to the symmetry property discussed in Section 3.3, a generalized momentum p_k conjugate to an ignorable coordinate is a constant. Therefore, according to this Lagrangian formulation of mechanics, a conserved quantity such as energy, momentum or angular momentum, is a direct consequence of symmetry.

Example 3.5 A block of mass m_1 is free to slide on a frictionless track, as sketched in Figure 3.2. Another particle of mass m_2 suspended by a light rod of length l is attached to the block. Find equations of motion for both bodies.

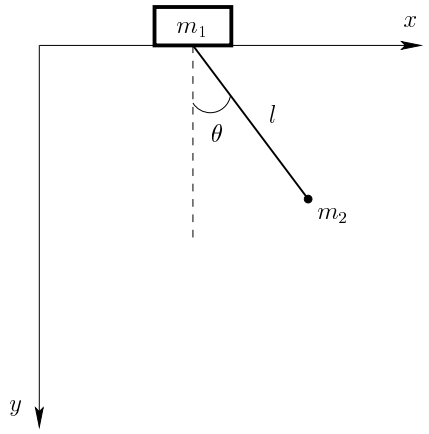


Figure 3.2: A pendulum suspended from a block moving on a frictionless surface.

Solution In this problem objects are characterized by three coordinates: the horizontal displacement of the block of mass m_1 is denoted by x_1; the position of the particle of mass m_2 is denoted by x_2 and y_2. Because the rod constrains the motion of the m_2, there remain only two degrees of freedom: the horizontal displacement x_1 of m_1, and the angular displacement θ of m_2. The transformation equations pertaining to the particle of mass m_2 are

$$x_2 = x_1 + l\sin\theta, \tag{3.32a}$$

$$y_2 = l\cos\theta. \tag{3.32b}$$

The kinetic energy of this system is

$$T = \frac{1}{2}m_1\dot{x_1}^2 + \frac{1}{2}m_2(\dot{x_2}^2 + \dot{y_2}^2),$$

and the potential energy is

$$V = -m_2 g y_2.$$

Using Maple to perform the calculations, the Lagrangian is expressed in generalized coordinates as

$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2(\dot{x}_1^2 + l^2\dot{\theta}^2 + 2l\dot{\theta}\dot{x}_1\cos\theta) + m_2 gl\cos\theta. \tag{3.33}$$

The equations of motion are obtained on invoking the Euler–Lagrange equation. In this problem there are two variables x_1 and θ. For x_1, we have

$$m_1\ddot{x}_1 + m_2\ddot{x}_1 - m_2 l\sin\theta\dot{\theta}^2 + m_2 l\cos\theta\ddot{\theta} = 0, \tag{3.34}$$

and for θ we find

$$\ddot{x}_1 \cos\theta + l\ddot{\theta} + g\sin\theta = 0. \tag{3.35}$$

The differential equations obtained from the Euler–Lagrange equation are typically coupled. To simplify these equations, we undertake rearrangements to decouple them. In this example, we obtain an equation of θ alone by eliminating x_1 in the above two equations,

$$\left(\frac{m_2 l\cos\theta}{m_1+m_2} - \frac{l}{\cos\theta}\right)\ddot{\theta} - \frac{m_2 l\sin\theta}{m_1+m_2}\dot{\theta}^2 - g\frac{\sin\theta}{\cos\theta} = 0. \tag{3.36}$$

To derive the differential equations is straightforward, although perhaps tedious, but to solve them is more difficult; we will discuss this point in Chapter 4.

Worksheet 3.9 In this worksheet, we first define the transformation equations to obtain the Lagrangian in generalized coordinates. We apply our customary technique to derive the equations of motion. `Eq7` concerns the x_1 coordinate, and `Eq17` concerns the θ coordinate. To eliminate the variable x_1, we isolate $\ddot{x}$ from `Eq7` and `Eq17` then equate their right-hand sides.

```
> x2 := x1(t) + l*sin(theta(t));
```

$$x2 := \mathrm{x1}(t) + l\sin(\theta(t))$$

```
> y2 := -l*cos(theta(t));
```

$$y2 := -l\cos(\theta(t))$$

```
> T := 1/2*m1*diff(x1(t),t)^2 + 1/2*m2*(diff(x2,t)^2 +
> diff(y2,t)^2);
```

$$T := \frac{1}{2}\,m1\,(\tfrac{d}{dt}\,\mathrm{x1}(t))^2 + \frac{1}{2}\,m2\,(((\tfrac{d}{dt}\,\mathrm{x1}(t)) + l\cos(\theta(t))\,(\tfrac{d}{dt}\,\theta(t)))^2 + l^2\sin(\theta(t))^2\,(\tfrac{d}{dt}\,\theta(t))^2)$$

```
> V := m2*g*y2;
```

$$V := -m2\,g\,l\cos(\theta(t))$$

```
> L := T - V:
> L := simplify(L);
```

$$L := \frac{1}{2}\,m1\,(\tfrac{d}{dt}\,\mathrm{x1}(t))^2 + \frac{1}{2}\,m2\,(\tfrac{d}{dt}\,\mathrm{x1}(t))^2 + m2\,(\tfrac{d}{dt}\,\mathrm{x1}(t))\,l\cos(\theta(t))\,(\tfrac{d}{dt}\,\theta(t)) + \frac{1}{2}\,m2\,l^2\,(\tfrac{d}{dt}\,\theta(t))^2 + m2\,g\,l\cos(\theta(t))$$

```
> L1 := subs({x1(t)=var1, diff(x1(t),t)=var2, theta(t)=var3,
> diff(theta(t),t)=var4}, L):
> Epr1 := diff(L1, var2):
> Epr2 := diff(L1, var1):
```

```
> Epr3 := subs({var1=x1(t), var2=diff(x1(t),t), var3=theta(t),
> var4=diff(theta(t),t)}, Epr1):
> Epr4 := subs({var1=x1(t), var2=diff(x1(t),t), var3=theta(t),
> var4=diff(theta(t),t)}, Epr2):
> Epr5 := diff(Epr3,t):
> Eq6 := Epr5 - Epr4 = 0:
> Eq7 := simplify(Eq6);
```

$$Eq7 := m1\,(\tfrac{d^2}{dt^2}\,\mathrm{x1}(t)) + m2\,(\tfrac{d^2}{dt^2}\,\mathrm{x1}(t)) - m2\,l\sin(\theta(t))\,(\tfrac{d}{dt}\,\theta(t))^2 + m2\,l\cos(\theta(t))\,(\tfrac{d^2}{dt^2}\,\theta(t)) = 0$$

```
> Epr11 := diff(L1, var4):
> Epr12 := diff(L1, var3):
> Epr13 := subs({var1=x1(t), var2=diff(x1(t),t), var3=theta(t),
> var4=diff(theta(t),t)}, Epr11):
> Epr14 := subs({var1=x1(t), var2=diff(x1(t),t), var3=theta(t),
> var4=diff(theta(t),t)}, Epr12):
> Epr15 := diff(Epr13,t):
> Eq16 := Epr15 - Epr14 = 0:
> Eq17 := simplify(Eq16);
```

$$Eq17 := m2\,l\,((\tfrac{d^2}{dt^2}\,\mathrm{x1}(t))\cos(\theta(t)) + l\,(\tfrac{d^2}{dt^2}\,\theta(t)) + g\sin(\theta(t))) = 0$$

```
> Eq21 := isolate(Eq7, diff(x1(t),t$2)):
> Eq22 := isolate(Eq17, diff(x1(t),t$2)):
> Eq23 := rhs(Eq21) = rhs(Eq22):
> Eq24 := collect(Eq23, diff);
```

$$Eq24 := \frac{m2\,l\sin(\theta(t))\,(\frac{d}{dt}\,\theta(t))^2}{m1+m2} - \frac{m2\,l\cos(\theta(t))\,(\frac{d^2}{dt^2}\,\theta(t))}{m1+m2} = -\frac{l\,(\frac{d^2}{dt^2}\,\theta(t))}{\cos(\theta(t))} - \frac{g\sin(\theta(t))}{\cos(\theta(t))}$$

3.6 Force of Constraint

In many physical situations, a particle is restricted to move on a surface; for example, a bead slides on a sphere. Under such a condition, there is a normal force exerted on the bead from

the surface, called the force of constraint. Our interest concerns a particular class of constraint, namely that in which the generalized coordinates are subject to l constraint equations of the form

$$f_i(q_1, q_2, \ldots, q_n, t) = 0, \quad i = 1, 2, \ldots, l. \tag{3.37}$$

Before formulating such a problem, we explain the principle of virtual work. Consider a dielectric slab partially inserted between two parallel plates maintained at a potential difference V, for which we seek to evaluate the force acting on the slab. To find the force directly is difficult, but to find the energy of the system is easy. We imagine that the material slides a little, and note the change in the energy; on differentiating the energy with respect to the displacement, we obtain the force. As the displacement exists only in our imagination, we describe it as a virtual displacement, and the energy change is the virtual work.

The Lagrangian formulation can be elegantly extended to include constraints. We introduce the Lagrange undetermined multipliers, denoted by λ_i, on constructing a modified Lagrangian

$$L' = L + \sum_{i=1}^{l} \lambda_i f_i. \tag{3.38}$$

The physical interpretation is that the extra terms represent the virtual work; because f_i can be considered a virtual displacement in the direction of the normal force, λ_i is the force of constraint.[2]

Example 3.6 A bead of mass m slides freely on a frictionless circular wire of radius a that rotates in a horizontal plane with constant angular velocity ω about a point; see Figure 3.3. Find the force of constraint acting on the bead.

Solution In addition to θ, we assume a degree of freedom r for the radial displacement. The equation expressing the constraint is

$$f = r(t) - a = 0. \tag{3.39}$$

The transformation equations are

$$x = a\cos\omega t + r\cos(\theta + \omega t), \quad y = a\sin\omega t + r\sin(\theta + \omega t). \tag{3.40}$$

The kinetic energy is

$$T = \frac{1}{2}(\dot{x}^2 + \dot{y}^2).$$

As there is no potential energy, the Lagrangian is

$$L = T = \frac{m}{2}[\dot{r}^2 + 2\dot{r}a\omega\sin\theta + a^2\omega^2 + r^2(\dot{\theta} + \omega)^2 + 2a\omega r(\dot{\theta} + \omega)\cos\theta]. \tag{3.41}$$

[2]Strictly speaking, λ_i itself might not be the force, but is related to the force in a simple way.

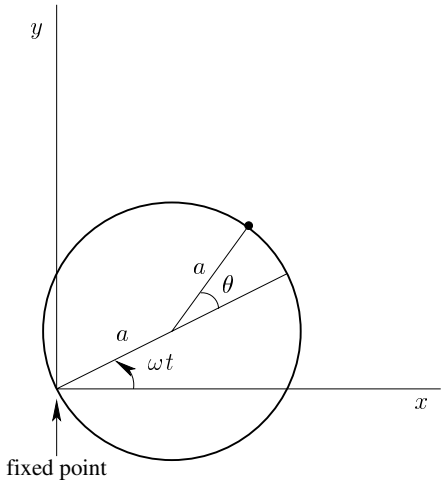


Figure 3.3: A bead sliding on a wire.

We form a function with an undetermined multiplier,

$$L' = L + \lambda(r - a), \tag{3.42}$$

and employ the Euler–Lagrange equation. For the r coordinate,

$$m\ddot{r} - ma\omega^2 \cos\theta - mr(\dot{\theta} + \omega)^2 - \lambda = 0, \tag{3.43}$$

and for θ,

$$2mr\dot{\theta}\dot{r} + mr^2\ddot{\theta} + 2mr\dot{r}\omega + ma\omega^2 r \sin\theta = 0. \tag{3.44}$$

According to the constraint,

$$r = a, \tag{3.45}$$

which we substitute into the equations that we obtained above, so as to produce

$$-ma\omega^2 \cos\theta - ma(\dot{\theta} + \omega)^2 - \lambda = 0.$$

The reactive force is thus solved:

$$\lambda = -ma(\dot{\theta} + \omega)^2 - ma\omega^2 \cos\theta. \tag{3.46}$$

Because r is fixed at a, $\dot{r} = 0$. The equation of motion for the θ coordinate becomes

$$\ddot{\theta} + \omega^2 \sin\theta = 0. \tag{3.47}$$

The motion of the bead on the wire is governed by an equation of exactly the same form as for a simple pendulum.

Worksheet 3.10 We first define the transformation equations for `x` and `y`, and use Maple to find the expression for kinetic energy in generalized coordinates. We employ the `combine` command which greatly simplifies an expression containing trigonometric functions. The techniques of using commands such as `subs`, `diff` and `isolate` are similar to those in preceding worksheets.

```
> x := a*cos(omega*t) + r(t)*cos(theta(t) + omega*t);
```

$$x := a\cos(\omega\, t) + \mathrm{r}(t)\cos(\theta(t) + \omega\, t)$$

```
> y := a*sin(omega*t) + r(t)*sin(theta(t) + omega*t);
```

$$y := a\sin(\omega\, t) + \mathrm{r}(t)\sin(\theta(t) + \omega\, t)$$

```
> T := 1/2*m*(diff(x,t)^2 + diff(y,t)^2);
```

$$T := \frac{1}{2}m((-a\sin(\omega\, t)\,\omega + (\tfrac{d}{dt}\,\mathrm{r}(t))\cos(\%1) - \mathrm{r}(t)\sin(\%1)\,((\tfrac{d}{dt}\,\theta(t)) + \omega))^2$$
$$+ (a\cos(\omega\, t)\,\omega + (\tfrac{d}{dt}\,\mathrm{r}(t))\sin(\%1) + \mathrm{r}(t)\cos(\%1)\,((\tfrac{d}{dt}\,\theta(t)) + \omega))^2)$$
$$\%1 := \theta(t) + \omega\, t$$

```
> L := simplify(T):
> L := combine(L);
```

$$L := \frac{m\,a^2\,\omega^2}{2} + m\,a\,\omega\,(\tfrac{d}{dt}\,\mathrm{r}(t))\sin(\theta(t)) + m\,a\,\omega\,\mathrm{r}(t)\,(\tfrac{d}{dt}\,\theta(t))\cos(\theta(t))$$
$$+ m\,a\,\omega^2\,\mathrm{r}(t)\cos(\theta(t)) + \frac{1}{2}\,m\,\mathrm{r}(t)^2\,(\tfrac{d}{dt}\,\theta(t))^2 + m\,\mathrm{r}(t)^2\,(\tfrac{d}{dt}\,\theta(t))\,\omega + \frac{1}{2}\,m\,\mathrm{r}(t)^2\,\omega^2$$
$$+ \frac{1}{2}\,m\,(\tfrac{d}{dt}\,\mathrm{r}(t))^2$$

```
> f := r(t) - a;
```

$$f := \mathrm{r}(t) - a$$

```
> Lp := L + lambda*f;
```

$$Lp := \frac{m\,a^2\,\omega^2}{2} + m\,a\,\omega\,(\tfrac{d}{dt}\,\mathrm{r}(t))\sin(\theta(t)) + m\,a\,\omega\,\mathrm{r}(t)\,(\tfrac{d}{dt}\,\theta(t))\cos(\theta(t))$$
$$+ m\,a\,\omega^2\,\mathrm{r}(t)\cos(\theta(t)) + \frac{1}{2}\,m\,\mathrm{r}(t)^2\,(\tfrac{d}{dt}\,\theta(t))^2 + m\,\mathrm{r}(t)^2\,(\tfrac{d}{dt}\,\theta(t))\,\omega + \frac{1}{2}\,m\,\mathrm{r}(t)^2\,\omega^2$$
$$+ \frac{1}{2}\,m\,(\tfrac{d}{dt}\,\mathrm{r}(t))^2 + \lambda\,(\mathrm{r}(t) - a)$$

```
> L1 := subs({r(t)=var1, diff(r(t),t)=var2, theta(t)=var3,
> diff(theta(t),t)=var4}, Lp):
> Epr11 := diff(L1, var2):
> Epr12 := diff(L1, var1):
> Epr13 := subs({var1=r(t), var2=diff(r(t),t), var3=theta(t),
> var4=diff(theta(t),t)}, Epr11):
```

```
> Epr14 := subs({var1=r(t), var2=diff(r(t),t), var3=theta(t),
> var4=diff(theta(t),t)}, Epr12):
> Epr15 := diff(Epr13, t):
> Eq16 := Epr15 - Epr14 =0;
```

$$Eq16 := m\,(\tfrac{d^2}{dt^2}\,\mathrm{r}(t)) - m\,a\,\omega^2\cos(\theta(t)) - m\,\mathrm{r}(t)\,(\tfrac{d}{dt}\,\theta(t))^2 - 2\,m\,\mathrm{r}(t)\,(\tfrac{d}{dt}\,\theta(t))\,\omega - m\,\mathrm{r}(t)\,\omega^2 - \lambda = 0$$

```
> Epr21 := diff(L1, var4):
> Epr22 := diff(L1, var3):
> Epr23 := subs({var1=r(t), var2=diff(r(t),t), var3=theta(t),
> var4=diff(theta(t),t)}, Epr21):
> Epr24 := subs({var1=r(t), var2=diff(r(t),t), var3=theta(t),
> var4=diff(theta(t),t)}, Epr22):
> Epr25 := diff(Epr23, t):
> Eq26 := Epr25 - Epr24 =0;
```

$$Eq26 := 2\,m\,\mathrm{r}(t)\,(\tfrac{d}{dt}\,\theta(t))\,(\tfrac{d}{dt}\,\mathrm{r}(t)) + m\,\mathrm{r}(t)^2\,(\tfrac{d^2}{dt^2}\,\theta(t)) + 2\,m\,\mathrm{r}(t)\,\omega\,(\tfrac{d}{dt}\,\mathrm{r}(t)) + m\,a\,\omega^2\,\mathrm{r}(t)\sin(\theta(t)) = 0$$

```
> Eq31 := f =0:
> Eq32 := isolate(Eq31, r(t));
```

$$Eq32 := \mathrm{r}(t) = a$$

```
> Eq41 := eval(Eq16, Eq32):
> Eq42 := eval(Eq26, Eq32):
> Eq43 := simplify(Eq41);
```

$$Eq43 := -m\,a\,\omega^2\cos(\theta(t)) - m\,a\,(\tfrac{d}{dt}\,\theta(t))^2 - 2\,m\,a\,(\tfrac{d}{dt}\,\theta(t))\,\omega - m\,a\,\omega^2 - \lambda = 0$$

```
> Eq44 := simplify(Eq42);
```

$$Eq44 := m\,a^2\,((\tfrac{d^2}{dt^2}\,\theta(t)) + \omega^2\sin(\theta(t))) = 0$$

```
> Eq45 := isolate(Eq43, lambda);
```

$$Eq45 := \lambda = -m\,a\,\omega^2\cos(\theta(t)) - m\,a\,(\tfrac{d}{dt}\,\theta(t))^2 - 2\,m\,a\,(\tfrac{d}{dt}\,\theta(t))\,\omega - m\,a\,\omega^2$$

We use another example to review the concept of conserved conjugate momentum and force of constraint.

Example 3.7 What is the motion of a particle moving under gravity if it is constrained to remain on the surface of a fixed solid sphere of radius a?

Solution It is convenient to use spherical coordinates. The kinetic energy in spherical coordinates is derived as in Section 1.5,

$$T = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2);$$

the potential energy is

$$V = mgz = mgr\cos\theta.$$

In this problem we express the constraint of r as

$$f = r - a = 0. \tag{3.48}$$

We form the modified Lagrangian

$$L' = L + \lambda f, \tag{3.49}$$

and apply the Euler–Lagrange equations. For the r coordinate,

$$m\ddot{r} - m(r\dot{\theta}^2 + r\sin^2\theta\dot{\phi}^2) + mg\cos\theta - \lambda = 0, \tag{3.50}$$

and for the θ coordinate,

$$2mr\dot{\theta}\dot{r} + mr^2\ddot{\theta} - mr^2\sin\theta\cos\theta\dot{\phi}^2 - mgr\sin\theta = 0. \tag{3.51}$$

For the ϕ coordinate, because the Lagrangian does not contain ϕ explicitly, we obtain a conserved quantity, denoted l,

$$mr^2\sin^2\theta\dot{\phi} = l. \tag{3.52}$$

Solving the constraint equation, we have

$$r = a, \tag{3.53}$$

which imposes the condition that the particle moves only on the sphere. We again rearrange the three coupled equations. First, we express $\dot{\phi}$ as

$$\dot{\phi} = \frac{l}{ma^2\sin^2\theta} \tag{3.54}$$

so that we can eliminate $\dot{\phi}$ from the other equations. The equation of motion for the r coordinate is simply the constraint of equation (3.53). The force of constraint is solved by

$$\lambda = mg\cos\theta - ma\dot{\theta}^2 - \frac{l^2}{ma^3\sin^2\theta}. \tag{3.55}$$

We decouple the θ equation:

$$\ddot{\theta} - \frac{l^2\cos\theta}{m^2a^4\sin^3\theta} - \frac{g\sin\theta}{a} = 0. \tag{3.56}$$

Worksheet 3.11 We modify the Lagrangian by including an equation of constraint. There are three degrees of freedom: `Eq6` concerns the r coordinate, `Eq16` concerns the θ coordinate, and `Eq24` concerns the ϕ coordinate, for which the conjugate momentum p_ϕ is conserved, denoted by `l`. The equation for r is readily solved in `Eq36`. To decouple equations, we isolate the part that we seek to eliminate to the left-hand side, and equate the right-hand sides of the equations.

```
> T := 1/2*m*(diff(r(t),t)^2 + r(t)^2*diff(theta(t),t)^2 +
> r(t)^2*sin(theta(t))^2*diff(phi(t),t)^2);
```

$$T := \frac{1}{2}\, m\, ((\tfrac{d}{dt}\, \mathrm{r}(t))^2 + \mathrm{r}(t)^2\, (\tfrac{d}{dt}\, \theta(t))^2 + \mathrm{r}(t)^2 \sin(\theta(t))^2\, (\tfrac{d}{dt}\, \phi(t))^2)$$

```
> V := m*g*r(t)*cos(theta(t));
```

$$V := m\, g\, \mathrm{r}(t) \cos(\theta(t))$$

```
> L := T-V;
```

$$L := \frac{1}{2}\, m\, ((\tfrac{d}{dt}\, \mathrm{r}(t))^2 + \mathrm{r}(t)^2\, (\tfrac{d}{dt}\, \theta(t))^2 + \mathrm{r}(t)^2 \sin(\theta(t))^2\, (\tfrac{d}{dt}\, \phi(t))^2) - m\, g\, \mathrm{r}(t) \cos(\theta(t))$$

```
> f := r(t)-a;
```

$$f := \mathrm{r}(t) - a$$

```
> Lc := L + lambda*f;
```

$$Lc := \frac{1}{2}\, m\, ((\tfrac{d}{dt}\, \mathrm{r}(t))^2 + \mathrm{r}(t)^2\, (\tfrac{d}{dt}\, \theta(t))^2 + \mathrm{r}(t)^2 \sin(\theta(t))^2\, (\tfrac{d}{dt}\, \phi(t))^2) - m\, g\, \mathrm{r}(t) \cos(\theta(t)) + \lambda\, (\mathrm{r}(t) - a)$$

```
> L1 := subs({r(t)=var1, diff(r(t),t)=var2, theta(t)=var3,
> diff(theta(t),t)=var4, phi(t)=var5, diff(phi(t),t)=var6}, Lc):
> Epr1 := diff(L1, var2):
> Epr2 := diff(L1, var1):
> Epr3 := subs({var1=r(t), var2=diff(r(t),t), var3=theta(t),
> var4=diff(theta(t),t), var5=phi(t), var6=diff(phi(t),t)}, Epr1):
> Epr4 := subs({var1=r(t), var2=diff(r(t),t), var3=theta(t),
> var4=diff(theta(t),t), var5=phi(t), var6=diff(phi(t),t)}, Epr2):
> Epr5 := diff(Epr3,t):
> Eq6 := Epr5 - Epr4 = 0;
```

$$Eq6 := m\, (\tfrac{d^2}{dt^2}\, \mathrm{r}(t)) - \frac{1}{2}\, m\, (2\, \mathrm{r}(t)\, (\tfrac{d}{dt}\, \theta(t))^2 + 2\, \mathrm{r}(t) \sin(\theta(t))^2\, (\tfrac{d}{dt}\, \phi(t))^2) + m\, g \cos(\theta(t)) - \lambda = 0$$

```
> Epr11 := diff(L1, var4):
> Epr12 := diff(L1, var3):
> Epr13 := subs({var1=r(t), var2=diff(r(t),t), var3=theta(t),
> var4=diff(theta(t),t), var5=phi(t), var6=diff(phi(t),t)}, Epr11):
> Epr14:=subs({var1=r(t), var2=diff(r(t),t), var3=theta(t),
> var4=diff(theta(t),t), var5=phi(t), var6=diff(phi(t),t)}, Epr12):
> Epr15 := diff(Epr13,t):
> Eq16 := Epr15 - Epr14 = 0;
```

$$Eq16 := 2\,m\,\mathrm{r}(t)\,(\tfrac{d}{dt}\,\theta(t))\,(\tfrac{d}{dt}\,\mathrm{r}(t)) + m\,\mathrm{r}(t)^2\,(\tfrac{d^2}{dt^2}\,\theta(t)) - m\,\mathrm{r}(t)^2\sin(\theta(t))\,(\tfrac{d}{dt}\,\phi(t))^2\cos(\theta(t)) - m\,g\,\mathrm{r}(t)\sin(\theta(t)) = 0$$

```
> Epr21 := diff(L1, var6):
> Epr22 := diff(L1, var5):
> Epr23 := subs({var1=r(t), var2=diff(r(t),t), var3=theta(t),
> var4=diff(theta(t),t), var5=phi(t), var6=diff(phi(t),t)}, Epr21):
> Epr24 := subs({var1=r(t), var2=diff(r(t),t), var3=theta(t),
> var4=diff(theta(t),t), var5=phi(t), var6=diff(phi(t),t)}, Epr22):
> Eq27 := Epr23 = l;
```

$$Eq27 := m\,\mathrm{r}(t)^2\sin(\theta(t))^2\,(\tfrac{d}{dt}\,\phi(t)) = l$$

```
> Eq35 := f = 0;
```

$$Eq35 := \mathrm{r}(t) - a = 0$$

```
> Eq36 := isolate(Eq35, r(t));
```

$$Eq36 := \mathrm{r}(t) = a$$

```
> Eq37 := eval(Eq6, Eq36);
```

$$Eq37 := -\frac{1}{2}\,m\,(2\,a\,(\tfrac{d}{dt}\,\theta(t))^2 + 2\,a\sin(\theta(t))^2\,(\tfrac{d}{dt}\,\phi(t))^2) + m\,g\cos(\theta(t)) - \lambda = 0$$

```
> Eq38 := eval(Eq16, Eq36);
```

$$Eq38 := m\,a^2\,(\tfrac{d^2}{dt^2}\,\theta(t)) - m\,a^2\sin(\theta(t))\,(\tfrac{d}{dt}\,\phi(t))^2\cos(\theta(t)) - m\,g\,a\sin(\theta(t)) = 0$$

```
> Eq39 := eval(Eq27, Eq36);
```

$$Eq39 := m\,a^2\sin(\theta(t))^2\,(\tfrac{d}{dt}\,\phi(t)) = l$$

```
> Eq41 := isolate(Eq39, diff(phi(t),t));
```

$$Eq41 := \tfrac{d}{dt}\,\phi(t) = \frac{l}{m\,a^2\sin(\theta(t))^2}$$

```
> Eq42 := eval(Eq37, Eq41);
```

$$Eq42 := -\frac{1}{2}\,m\,\left(2\,a\,(\tfrac{d}{dt}\,\theta(t))^2 + \frac{2\,l^2}{a^3\sin(\theta(t))^2\,m^2}\right) + m\,g\cos(\theta(t)) - \lambda = 0$$

```
> Eq43 := isolate(Eq42, lambda);
```

$$Eq43 := \lambda = -\frac{1}{2}\,m\,\left(2\,a\,(\tfrac{d}{dt}\,\theta(t))^2 + \frac{2\,l^2}{a^3\sin(\theta(t))^2\,m^2}\right) + m\,g\cos(\theta(t))$$

```
> Eq44 := eval(Eq38, Eq41);
```

$$Eq44 := m\,a^2\,(\tfrac{d^2}{dt^2}\,\theta(t)) - \frac{l^2\cos(\theta(t))}{m\,a^2\sin(\theta(t))^3} - m\,g\,a\sin(\theta(t)) = 0$$

The reader is encouraged to read Chapter 19 of *The Feynman Lectures*, vol. 2, in which Richard Feynman described how he became fascinated by the principle of least action. Exploiting this simple idea, he proceeded to formulate his famous space–time approach to quantum mechanics. In addition to his physical intuition, Feynman possessed an extraordinary ability to calculate, which is essential in the evaluation of cumbersome path integrals. Although this topic is beyond our scope, we remind the reader to make optimum use of computer algebra to enhance productivity. The first three exercises below provide basic but important results useful for path integrals, and we will encounter them again in exercises for quantum mechanics in Chapters 14 and 15.

Exercises

1. For a free particle of mass m in one dimension, the Lagrangian is simply

$$L = \frac{1}{2}m\dot{x}^2. \tag{3.57}$$

   (a) Derive the equation of motion for this particle.

   (b) Suppose that the particle moves from point x_a at time t_a to point x_b at time t_b; solve the equation of motion under those conditions to obtain x as a function of t.

   (c) Show that the minimal action, i.e., the time integral of the Lagrangian from $t = t_a$ to $t = t_b$ is

$$S = \int_{t_a}^{t_b} L\,dt = \frac{m}{2}\frac{(x_b - x_a)^2}{t_b - t_a}. \tag{3.58}$$

2. For a particle of mass m in one dimension under the influence of gravity, the Lagrangian is

$$L = \frac{1}{2}m\dot{x}^2 - mgx. \tag{3.59}$$

   (a) Derive the equation of motion for this particle.

(b) Solve the equation of motion for the particle to move from x_a at $t = 0$ to x_b at $t = t_b$.

(c) Show that the minimal action in that motion from $t = 0$ to $t = t_b$ is

$$S = \int_0^{t_b} L\,dt = \frac{m}{2}\frac{(x_b - x_a)^2}{2t_b} - \frac{mg}{2}t_b(x_b + x_a) - \frac{1}{24}mg^2t_b^3. \tag{3.60}$$

3. For a particle of mass m under the influence of a linear restoring force, the Lagrangian is

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2. \tag{3.61}$$

(a) Derive the equation of motion for this particle.

(b) For this particle subject to boundary conditions $x(0) = x_a$ and $x(t_b) = x_b$, solve for $x(t)$.

(c) Show that the minimal action for motion from $t = 0$ to $t = t_b$ is

$$S = \int_0^{t_b} L\,dt = \frac{m\omega}{2\sin(\omega t_b)}[(x_a^2 + x_b^2)\cos(\omega t_b) - 2x_a x_b]. \tag{3.62}$$

4. For an integral

$$T = \int_0^{x_1} \frac{\sqrt{1 + \left[\frac{d}{dx}z(x)\right]^2}}{[z(x) + z_0]}\,dx, \tag{3.63}$$

derive the differential equation that the function $z(x)$ must satisfy, so that T has an extremal; find the solutions for $z(x)$.

5. Derive the Euler–Lagrange equation to describe a brachistochrone curve for a particle moving inside a spherical planet of uniform mass density.

6. A bead of mass m is constrained to move on a vertical hoop of radius a, rotating at angular velocity ω. Derive the Lagrangian for the bead and the equation of motion.

7. A thin rod of length $2a$ and mass m is connected, at one end, to a vertical axis rotating at angular velocity ω, see Figure 3.4. Assuming that the rod subtends an angle θ with the axis, derive the Lagrangian and equation of motion for θ.

Hint: the only degree of freedom is θ; the transformations are

$$x = r\sin\theta\cos\omega t, \quad y = r\sin\theta\sin\omega t, \quad z = 2a - r\cos\theta.$$

The kinetic energy is obtained on integrating

$$dT = \frac{1}{2}(dm)(\dot{x}^2 + \dot{y}^2 + \dot{z}^2), \quad dm = \frac{m}{2a}dr,$$

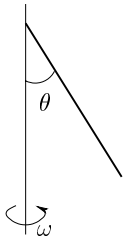


Figure 3.4: A rod of length $2a$ rotates around a vertical axis.

and the potential energy from

$$dV = (dm)gz.$$

8. A particle of mass m is connected by a massless spring of force constant k and unstressed length r_0 to a point P that is moving along a horizontal circular path of radius a at a uniform angular velocity ω, see Figure 3.5. Show that the Lagrangian for this system is

$$L = \frac{1}{2}m[\dot{r}^2 + a^2\omega^2 + r\dot{\theta}^2 + 2a\omega\dot{r}\sin(\theta - \omega t) + 2a\omega r\dot{\theta}\cos(\theta - \omega t)] - \frac{1}{2}k(r - r_0)^2. \tag{3.64}$$

Derive the equations of motion for r and θ.

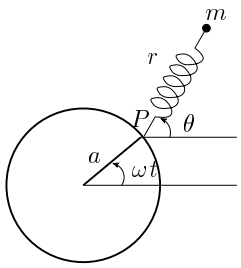


Figure 3.5: A particle connected to a rotating point by a spring.

Hint: let the coordinate of P be $(x_1, y_1) = (\cos\omega t, \sin\omega t)$, and that of the particle be $(x_2, y_2) = (x_1 + r\cos\theta, y_1 + r\sin\theta)$, then $T = \frac{1}{2}m(\dot{x_2}^2 + \dot{y_2}^2)$.

9. A particle of mass m is placed at the top of a vertical hoop of radius a; see Figure 3.6. Calculate the reaction of the hoop on the particle by means of the Lagrange undetermined multipliers and the Euler–Lagrange equation, and find the point at which the particle falls off.

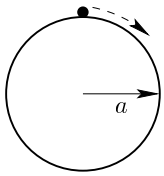


Figure 3.6: A particle placed at the top of a hoop.

Hint: to find the point at which the particle falls off, one needs to use the fact that $T + V$ is conserved.

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4 Integration of Equations of Motion

In Chapter 3 we derived the equations of motion by employing the Euler–Lagrange equation. As most differential equations admit no analytic solution, in this chapter we first introduce the small-angle approximation so that we can linearize differential equations to obtain analytic solutions. In the rest of the chapter we tackle most problems using numerical methods. It is not our purpose to treat those problems formally, because such an approach can be found in numerous books. We exploit Maple's ability to solve equations numerically and to produce plots based on numerical solutions. Our emphasis is on experimenting with various numerical assignments and viewing the outcome so as to develop physical insight.

4.1 Linearization of Equations

In the example in Section 3.5, we have a pendulum suspended from a block that is confined to move on a frictionless surface. We have derived the equations of motion; after further simplification we obtained a decoupled equation for the θ coordinate,

$$\left(\frac{m_2 l\cos\theta}{m_1+m_2}-\frac{l}{\cos\theta}\right)\ddot{\theta}-\frac{m_2 l\sin\theta}{m_1+m_2}\dot{\theta}^2-g\frac{\sin\theta}{\cos\theta}=0. \tag{4.1}$$

This equation has no exact analytic solution, but, if the amplitude of oscillation is small – that is when $|\theta|\ll 1$, we can apply the small-angle approximation:

$$\sin\theta\cong\theta, \tag{4.2}$$

and

$$\cos\theta\cong 1. \tag{4.3}$$

Furthermore, we can discard terms to higher powers such as $\dot{\theta}^2$. This technique is commonly used in approximation. With these preparations, equation (4.1) becomes a linear equation,

$$\ddot{\theta}=-\frac{g}{l}\frac{m_1+m_2}{m_1}\theta. \tag{4.4}$$

Its solution is

$$\theta=c_1\sin\left(\sqrt{\frac{g}{l}\frac{m_1+m_2}{m_1}}t\right)+c_2\cos\left(\sqrt{\frac{g}{l}\frac{m_1+m_2}{m_1}}t\right). \tag{4.5}$$

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Worksheet 4.1 In this worksheet we use the `subs` command to substitute $\sin\theta$ with θ, $\cos\theta$ with 1, and $\dot{\theta}^2$ with 0. To solve the linear differential equation, we use `dsolve` .

```
> Eq1 := (m2*l*cos(theta(t))/(m1+m2) -
> l/cos(theta(t)))*diff(theta(t),t$2) -
> m2*l*sin(theta(t))/(m1+m2)*diff(theta(t),t)^2 -
> g*sin(theta(t))/cos(theta(t)) = 0;
```

$$Eq1 := \left(\frac{m2\,l\cos(\theta(t))}{m1+m2} - \frac{l}{\cos(\theta(t))}\right)\left(\frac{d^2}{dt^2}\theta(t)\right) - \frac{m2\,l\sin(\theta(t))\left(\frac{d}{dt}\theta(t)\right)^2}{m1+m2} - \frac{g\sin(\theta(t))}{\cos(\theta(t))} = 0$$

```
> Eq2 := subs({cos(theta(t))=1, sin(theta(t))=theta(t)}, Eq1);
```

$$Eq2 := \left(\frac{m2\,l}{m1+m2} - l\right)\left(\frac{d^2}{dt^2}\theta(t)\right) - \frac{m2\,l\,\theta(t)\left(\frac{d}{dt}\theta(t)\right)^2}{m1+m2} - g\,\theta(t) = 0$$

```
> Eq3 := subs(diff(theta(t),t)^2=0, Eq2);
```

$$Eq3 := \left(\frac{m2\,l}{m1+m2} - l\right)\left(\frac{d^2}{dt^2}\theta(t)\right) - g\,\theta(t) = 0$$

```
> Eq4 := isolate(Eq3, diff(theta(t),t$2)):
> Eq5 := simplify(Eq4);
```

$$Eq5 := \frac{d^2}{dt^2}\theta(t) = -\frac{g\,\theta(t)\,(m1+m2)}{l\,m1}$$

```
> Soln1 := dsolve(Eq5, theta(t));
```

$$Soln1 := \theta(t) = _C1\sin\left(\frac{\sqrt{g}\,\sqrt{m1+m2}\,t}{\sqrt{l}\,\sqrt{m1}}\right) + _C2\cos\left(\frac{\sqrt{g}\,\sqrt{m1+m2}\,t}{\sqrt{l}\,\sqrt{m1}}\right)$$

4.2 Double Pendulum

The problem of a double pendulum is a classic example of the Lagrangian formulation of mechanics. The coordinates are defined in Figure 4.1; the y axis is taken to be positive downwards.

The position of a bob of mass m_1 in Cartesian coordinates is x_1 and y_1; the position of another bob of m_2 is x_2 and y_2. These Cartesian coordinates are not, however, independent of each other. A double pendulum has two degrees of freedom, and it is appropriate to use two

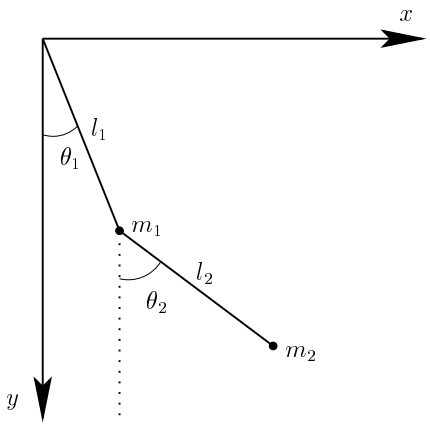


Figure 4.1: Double pendulum.

generalized coordinates: θ_1 and θ_2. The transformation equations are

$$x_1 = l_1 \sin\theta_1, \quad y_1 = l_1 \cos\theta_1, \tag{4.6a}$$

and

$$x_2 = x_1 + l_2 \sin\theta_2, \quad y_2 = y_1 + l_2 \cos\theta_2. \tag{4.6b}$$

In Cartesian coordinates, the kinetic energy is

$$T = \frac{1}{2} m_1 (\dot{x}_1^2 + \dot{y}_1^2) + \frac{1}{2} m_2 (\dot{x}_2^2 + \dot{y}_2^2),$$

and the potential energy is

$$V = -m_1 g y_1 - m_2 g y_2.$$

From the transformation equations, we obtain the Lagrangian in generalized coordinates:

$$L = \frac{1}{2} m_1 l_1^2 \dot{\theta}_1^2 + \frac{1}{2} m_2 [l_1^2 \dot{\theta}_1^2 + l_2^2 \dot{\theta}_2^2 + 2 l_1 l_2 \dot{\theta}_1 \dot{\theta}_2 \cos(\theta_1 - \theta_2)] + m_1 g l_1 \cos\theta_1 + m_2 g (l_1 \cos\theta_1 + l_2 \cos\theta_2). \tag{4.7}$$

Employing the Euler–Lagrange equation, we obtain for θ_1,

$$(m_1+m_2) l_1^2 \ddot{\theta}_1 + m_2 l_1 l_2 \cos(\theta_1-\theta_2) \ddot{\theta}_2 + m_2 l_1 l_2 \sin(\theta_1-\theta_2) \dot{\theta}_2^{\,2} + (m_1+m_2) g l_1 \sin\theta_1 = 0, \tag{4.8}$$

and for θ_2,

$$m_2 l_1 l_2 \cos(\theta_1 - \theta_2) \ddot{\theta}_1 + m_2 l_2^2 \ddot{\theta}_2 - m_2 l_1 l_2 \sin(\theta_1 - \theta_2) \dot{\theta}_1^{\,2} + m_2 g l_2 \sin\theta_2 = 0. \tag{4.9}$$

These two coupled differential equations admit no exact solution. One might apply the small-angle approximation to linearize the equations and to obtain the normal modes; see an exercise at the end of the chapter. Here we apply Maple in order to solve the equations numerically. With this approach we need to provide four initial conditions for two second-order equations: they are values for $\theta_1(0)$, $\theta_2(0)$, $\dot{\theta}_1(0)$, and $\dot{\theta}_2(0)$.

Worksheet 4.2 We first define `x1`, `y1`, `x2` and `y2` according to the transformation equations, then use Maple to simplify the kinetic and potential energy in generalized coordinates; the `combine` command is exceedingly useful for this purpose. By this stage the derivation of equations of motion should be familiar: `Eq17` concerns the θ_1 coordinate, and `Eq27` the θ_2 coordinate. We assign suitable numerical values to mass, length and acceleration due to gravity. We then provide initial conditions, and use the `dsolve` command with the `numeric` option to solve the differential equations. To present the numerical solution graphically, we use the `odeplot` command from the `plots` package; we also use the method of producing a trajectory in the phase space first seen in Section 2.4.

```
> x1 := l1*sin(theta1(t));
```

$$x1 := l1 \sin(\theta1(t))$$

```
> y1 := l1*cos(theta1(t));
```

$$y1 := l1 \cos(\theta1(t))$$

```
> x2 := x1 + l2*sin(theta2(t));
```

$$x2 := l1 \sin(\theta1(t)) + l2 \sin(\theta2(t))$$

```
> y2 := y1 + l2*cos(theta2(t));
```

$$y2 := l1 \cos(\theta1(t)) + l2 \cos(\theta2(t))$$

```
> T := 1/2*m1*(diff(x1,t)^2 + diff(y1,t)^2) + 1/2*m2*(diff(x2,t)^2
+ diff(y2,t)^2):
> T := combine(T);
```

$$T := \frac{1}{2} m1\ l1^2 \left(\frac{d}{dt}\theta1(t)\right)^2 + \frac{1}{2} m2\ l1^2 \left(\frac{d}{dt}\theta1(t)\right)^2$$
$$+ m2\ l1 \left(\frac{d}{dt}\theta1(t)\right) l2 \left(\frac{d}{dt}\theta2(t)\right) \cos(\theta1(t) - \theta2(t)) + \frac{1}{2} m2\ l2^2 \left(\frac{d}{dt}\theta2(t)\right)^2$$

```
> V := -m1*g*y1 - m2*g*y2;
```

$$V := -m1\ g\ l1 \cos(\theta1(t)) - m2\ g\ (l1 \cos(\theta1(t)) + l2 \cos(\theta2(t)))$$

```
> L := T - V;
```

$$L := \frac{1}{2} m1\ l1^2 \left(\frac{d}{dt}\theta1(t)\right)^2 + \frac{1}{2} m2\ l1^2 \left(\frac{d}{dt}\theta1(t)\right)^2$$
$$+ m2\ l1 \left(\frac{d}{dt}\theta1(t)\right) l2 \left(\frac{d}{dt}\theta2(t)\right) \cos(\theta1(t) - \theta2(t)) + \frac{1}{2} m2\ l2^2 \left(\frac{d}{dt}\theta2(t)\right)^2$$
$$+ m1\ g\ l1 \cos(\theta1(t)) + m2\ g\ (l1 \cos(\theta1(t)) + l2 \cos(\theta2(t)))$$

```
> L1 := subs({theta1(t)=var1, diff(theta1(t), t)=var2,
> theta2(t)=var3, diff(theta2(t), t)=var4}, L):
> Epr11 := diff(L1, var2):
> Epr12 := diff(L1, var1):
> Epr13 := subs({var1=theta1(t), var2=diff(theta1(t), t),
> var3=theta2(t), var4=diff(theta2(t), t)}, Epr11):
> Epr14 := subs({var1=theta1(t), var2=diff(theta1(t), t),
> var3=theta2(t), var4=diff(theta2(t), t)}, Epr12):
> Epr15 := diff(Epr13, t):
> Eq16 := Epr15 - Epr14 = 0:
> Eq17 := collect(Eq16, diff);
```

$$Eq17 := m2\ l1\ l2 \sin(\theta1(t) - \theta2(t)) \left(\frac{d}{dt}\theta2(t)\right)^2 + (m2\ {l1}^2 + m1\ {l1}^2) \left(\frac{d^2}{dt^2}\theta1(t)\right) + m1\ g\ l1 \sin(\theta1(t)) + m2\ l1\ l2 \left(\frac{d^2}{dt^2}\theta2(t)\right) \cos(\theta1(t) - \theta2(t)) + m2\ g\ l1 \sin(\theta1(t)) = 0$$

```
> Epr21 := diff(L1, var4):
> Epr22 := diff(L1, var3):
> Epr23 := subs({var1=theta1(t), var2=diff(theta1(t), t),
> var3=theta2(t), var4=diff(theta2(t), t)}, Epr21):
> Epr24 := subs({var1=theta1(t), var2=diff(theta1(t), t),
> var3=theta2(t), var4=diff(theta2(t), t)}, Epr22):
> Epr25 := diff(Epr23, t):
> Eq26 := Epr25 - Epr24 = 0:
> Eq27 := collect(Eq26, diff);
```

$$\begin{aligned} Eq27 := {} & m2\ l1 \left(\frac{d^2}{dt^2}\theta1(t)\right) l2 \cos(\theta1(t) - \theta2(t)) \\ & - m2\ l1\ l2 \sin(\theta1(t) - \theta2(t)) \left(\frac{d}{dt}\theta1(t)\right)^2 \\ & + m2\ {l2}^2 \left(\frac{d^2}{dt^2}\theta2(t)\right) + m2\ g\ l2 \sin(\theta2(t)) = 0 \end{aligned}$$

```
> m1:=0.05; m2:=0.05; l1:=0.5; l2:=0.5; g:=9.8;
```

$$\begin{aligned} m1 &:= 0.05 \\ m2 &:= 0.05 \\ l1 &:= 0.5 \\ l2 &:= 0.5 \\ g &:= 9.8 \end{aligned}$$

```
> ini:=theta1(0)=Pi/2.0, D(theta1)(0)=0, theta2(0)=Pi/4.0,
> D(theta2)(0)=0; # choose your values
```

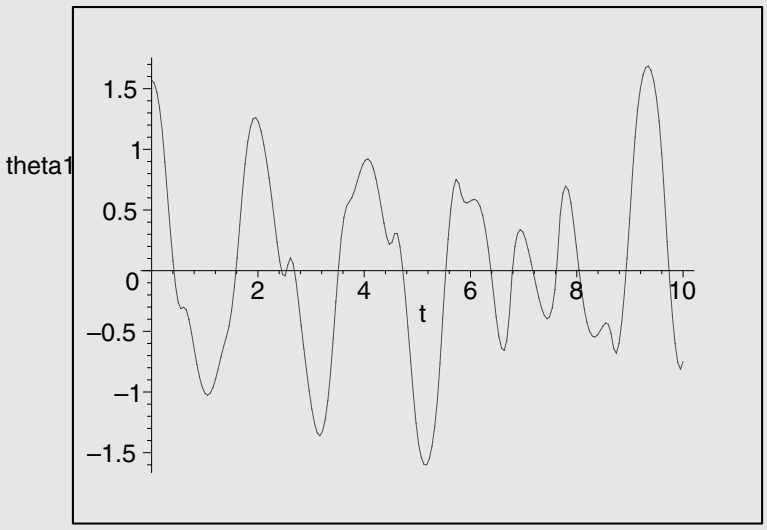
$$ini := \theta1(0) = 0.5000000000\,\pi, \mathrm{D}(\theta1)(0) = 0, \theta2(0) = 0.2500000000\,\pi, \mathrm{D}(\theta2)(0) = 0$$

```
> Eq75 := dsolve({Eq17, Eq27, ini}, {theta1(t), theta2(t)},
> numeric, output=listprocedure);
```

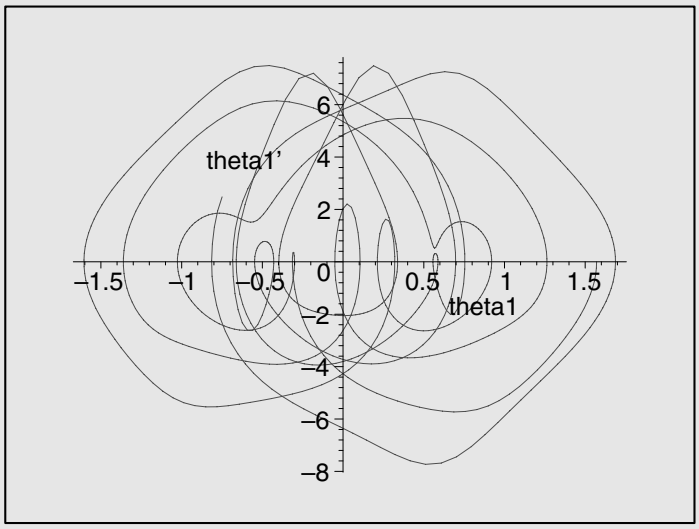
$$Eq75 := [t = (\textbf{proc}(t) \ldots \textbf{end proc}), \theta1(t) = (\textbf{proc}(t) \ldots \textbf{end proc}),$$
$$\tfrac{d}{dt}\theta1(t) = (\textbf{proc}(t) \ldots \textbf{end proc}), \theta2(t) = (\textbf{proc}(t) \ldots \textbf{end proc}),$$
$$\tfrac{d}{dt}\theta2(t) = (\textbf{proc}(t) \ldots \textbf{end proc})]$$

```
> with(plots): with(plottools):
Warning, the name changecoords has been redefined
Warning, the name arrow has been redefined

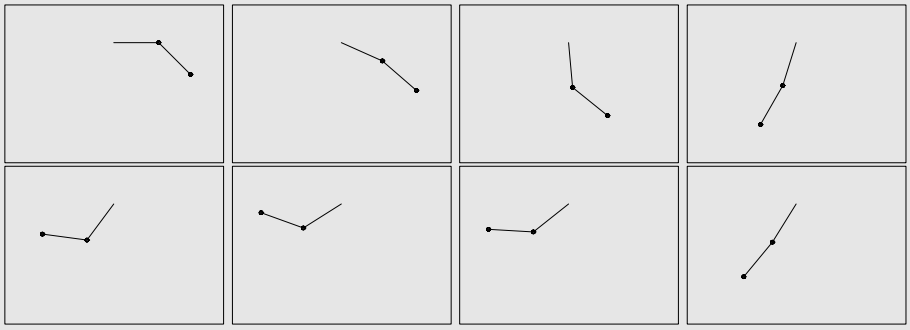
> odeplot(Eq75, [t, theta1(t)], 0..10, numpoints=200);
```




```
> odeplot(Eq75, [theta1(t), diff(theta1(t),t)], 0..10,
> numpoints=800);
```




```
> noffm:=100:  divs:=10:
> for i from 0 by 1 to noffm do
> x1 := l1*sin(rhs(Eq75[2](i/divs))):  y1 :=
> -l1*cos(rhs(Eq75[2](i/divs))):
> x2:=x1 + l2*sin(rhs(Eq75[4](i/divs))):  y2:= y1 -
> l2*cos(rhs(Eq75[4](i/divs))):
> rod[i]:=curve([[0,0], [x1,y1], [x2,y2]]):
> ms1[i]:=disk([x1,y1], 0.02, color=red):
> ms2[i]:=disk([x2,y2], 0.02, color=blue):
> anima[i]:=display({rod[i],ms1[i],ms2[i]}):
> end do:
> display([seq(anima[i],i=0..noffm)],insequence=true,
> scaling=constrained,axes=none);
```



In this example we deliberately choose large angles for our initial conditions. The resulting motion appears chaotic; this phenomenon is particularly pronounced from the trajectory in the phase space. We list the code for a simple animation that allows direct observation of the motion; because the representation of an animation on a printed page is awkward, we encourage the reader to run the program and to experiment with various initial conditions.

4.3 Central-force Problem

Consider a system of two mass points m_1 and m_2, where the only forces are those due to their mutual interaction. Such a two-body problem can be reduced to an equivalent problem, with one body of infinite mass fixed in space and the other body of reduced mass,

$$\mu = \frac{m_1 m_2}{m_1 + m_2}, \tag{4.10}$$

moving in space. We generally simply use a symbol m instead of μ, with the understanding that it indicates the reduced mass. If the potential energy V only depends on the mutual separation r of the two bodies, we describe such a force as a central force (because the force is always along $\mathbf{r}$). To treat a central-force problem, polar coordinates are convenient. One can prove that the two bodies remain in the same plane. Let the plane be $\theta = \pi/2$; according to our derivation in Section 1.5, the kinetic energy in polar coordinates is

$$T = \frac{1}{2} m(\dot{r}^2 + r^2 \dot{\phi}^2). \tag{4.11}$$

The Lagrangian is then

$$L = \frac{1}{2} m(\dot{r}^2 + r^2 \dot{\phi}^2) - V(r). \tag{4.12}$$

This Lagrangian has no explicit dependence on ϕ. Because of the symmetry property, the corresponding conjugate momentum, namely angular momentum, is a conserved quantity of the system:

$$p_\phi = \frac{\partial L}{\partial \dot{\phi}} \equiv l = \text{constant}. \tag{4.13}$$

Although we do not derive it, we state an important theorem: if a Lagrangian has no explicit dependence on time, the energy of the system is conserved:

$$\frac{\partial L}{\partial t} = 0, \quad T + V = E = \text{constant}. \tag{4.14}$$

Conserved quantities in mechanics, such as angular momentum and energy, are direct consequences of symmetries of the Lagrangian.

4.3.1 Kepler Problem

The most important central-force problem is one involving a force proportional to the inverse square of the distance – the Kepler problem. Newton's law of gravitation is

$$\mathbf{F} = -\frac{GMm}{r^2}\hat{\mathbf{r}}; \tag{4.15}$$

the potential energy is therefore

$$V = -\frac{GMm}{r}. \tag{4.16}$$

After forming the Lagrangian for the Kepler problem,

$$L = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\phi}^2) + \frac{GMm}{r}, \tag{4.17}$$

we obtain equations of motion. For ϕ,

$$mr^2\dot{\phi} = l, \tag{4.18}$$

where l is the constant angular momentum, and for r,

$$m\ddot{r} - mr\dot{\phi}^2 + \frac{GMm}{r^2} = 0. \tag{4.19}$$

We can solve these two equations numerically if initial conditions are provided; we need r_0, ϕ_0, $\dot{r}_0$, and $\dot{\phi}_0$. It is generally convenient to set zero time at the moment that $\dot{r} = 0$, and to define $\phi_0 = 0$.

To make the equations of motion easier to analyze, we decouple these two equations to obtain equations of r and ϕ separately:

$$\dot{\phi} = \frac{l}{mr^2}, \tag{4.20}$$

$$m\ddot{r} - \frac{l^2}{mr^3} + \frac{GMm}{r^2} = 0. \tag{4.21}$$

In our approach to the Kepler problem above, we made no use of the fact that energy is conserved; we simply obtain equations of motion from the Lagrangian, and directly solve those differential equations (numerically). Conservation of energy is a consequence of a symmetry property of the Lagrangian – its independence of time. As discussed in Section 3.3, we exploit symmetry to simplify calculations, so that a second-order differential equation is reduced to a first-order one. If we treat a mechanical problem as a problem of the calculus of variations, no knowledge about the energy is necessary: to find particle motion, we only need initial conditions.

Energy and angular momentum are, nevertheless, related to initial conditions. Because both energy and angular momentum are conserved, their values calculated from time zero remain invariant:

$$E = \frac{1}{2}m(\dot{r}_0^2 + r_0^2\dot{\phi}_0^2) + V(r_0), \tag{4.22}$$

and

$$l = mr_0^2\dot{\phi}_0. \tag{4.23}$$

In this worksheet we select various initial conditions and observe the orbit.

Worksheet 4.3 The derivation of equations of motion follows the same approach that we have used repeatedly: `Eq14` concerns the ϕ coordinate; the angular momentum is denoted `l`. `Eq26` concerns the r coordinate. We decouple two equations in `Eq31` and `Eq32`. To solve equations numerically and to make a plot, we set constants, such as G, M and m, to unity. For four required initial conditions, we supply r_0, $\dot{r}_0$, ϕ_0 and $\dot{\phi}_0$. Because we solve `Eq31` and `Eq32`, we must evaluate `l` from initial conditions. It is practical to solve `Eq14` and `Eq26` instead of obtaining the same trajectory, with the appropriate initial conditions supplied. To produce plots of functions in parametric form in polar coordinates, we use the `polarplot` command from the `plots` package.

```
> T := 1/2*m*(diff(r(t),t)^2 + r(t)^2*diff(phi(t),t)^2);
```

$$T := \frac{1}{2}\,m\,((\tfrac{d}{dt}\,\mathrm{r}(t))^2 + \mathrm{r}(t)^2\,(\tfrac{d}{dt}\,\phi(t))^2)$$

```
> V := -G*M*m/r(t);
```

$$V := -\frac{G\,M\,m}{\mathrm{r}(t)}$$

```
> L := T - V;
```

$$L := \frac{1}{2}\,m\,((\tfrac{d}{dt}\,\mathrm{r}(t))^2 + \mathrm{r}(t)^2\,(\tfrac{d}{dt}\,\phi(t))^2) + \frac{G\,M\,m}{\mathrm{r}(t)}$$

```
> L1 := subs({r(t)=var1, diff(r(t),t)=var2, phi(t)=var3,
> diff(phi(t),t)=var4}, L):
> Epr11 := diff(L1, var4):
> Epr12 := diff(L1, var3):
> Epr13 := subs({var1=r(t), var2=diff(r(t),t), var3=phi(t),
> var4=diff(phi(t),t)}, Epr11):
> Eq14 := Epr13 = l;
```

$$Eq14 := m\,\mathrm{r}(t)^2\,(\tfrac{d}{dt}\,\phi(t)) = l$$

```
> Epr21 := diff(L1, var2):
> Epr22 := diff(L1, var1):
```

```
> Epr23 := subs({var1=r(t), var2=diff(r(t),t), var3=phi(t),
> var4=diff(phi(t),t)}, Epr21):
> Epr24 := subs({var1=r(t), var2=diff(r(t),t), var3=phi(t),
> var4=diff(phi(t),t)}, Epr22):
> Epr25 := diff(Epr23,t):
> Eq26 := Epr25 - Epr24 = 0;
```

$$Eq26 := m\,(\tfrac{d^2}{dt^2}\,\mathrm{r}(t)) - m\,\mathrm{r}(t)\,(\tfrac{d}{dt}\,\phi(t))^2 + \frac{G\,M\,m}{\mathrm{r}(t)^2} = 0$$

```
> Eq31 := isolate(Eq14, diff(phi(t),t));
```

$$Eq31 := \tfrac{d}{dt}\,\phi(t) = \frac{l}{m\,\mathrm{r}(t)^2}$$

```
> Eq32 := eval(Eq26, Eq31);
```

$$Eq32 := m\,(\tfrac{d^2}{dt^2}\,\mathrm{r}(t)) - \frac{l^2}{m\,\mathrm{r}(t)^3} + \frac{G\,M\,m}{\mathrm{r}(t)^2} = 0$$

```
> with(plots):
Warning, the name changecoords has been redefined
> G:=1; M:=1; m:=1;
```

$$G := 1$$
$$M := 1$$
$$m := 1$$

```
> Eq41 := r(0) = 1;
```

$$Eq41 := \mathrm{r}(0) = 1$$

```
> Eq42 := D(r)(0) = 0;
```

$$Eq42 := \mathrm{D}(r)(0) = 0$$

```
> Eq43 := phi(0) = 0;
```

$$Eq43 := \phi(0) = 0$$

```
> Eq44 := D(phi)(0) = 1;
```

$$Eq44 := \mathrm{D}(\phi)(0) = 1$$

```
> En := eval(T + V, {r(t)=rhs(Eq41), diff(r(t),t)=rhs(Eq42),
> diff(phi(t),t)=rhs(Eq44)});
```

$$En := \frac{-1}{2}$$

```
> l := eval(lhs(Eq14), {r(t)=rhs(Eq41),
> diff(phi(t),t)=rhs(Eq44)});
```

$$l := 1$$

```
> epsilon := sqrt(1 + 2*En*l^2/(m*(G*M*m)^2));
```

$$\varepsilon := 0$$

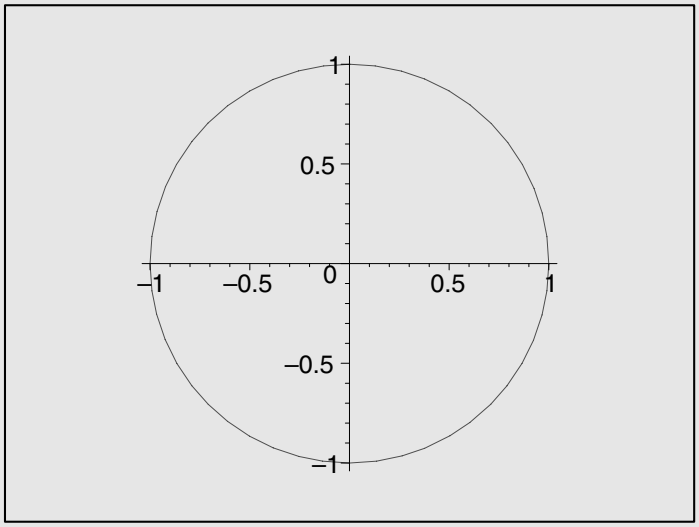
```
> ini1 := Eq41, Eq42, Eq43;
```

$$ini1 := \mathrm{r}(0) = 1, \mathrm{D}(r)(0) = 0, \phi(0) = 0$$

```
> Eq51:=dsolve({Eq31, Eq32, ini1}, {r(t), phi(t)}, numeric,
> output=listprocedure);
```

$$Eq51 := [t = (\mathbf{proc}(t) \ldots \mathbf{end\ proc}), \phi(t) = (\mathbf{proc}(t) \ldots \mathbf{end\ proc}),$$
$$\mathrm{r}(t) = (\mathbf{proc}(t) \ldots \mathbf{end\ proc}), \tfrac{d}{dt}\mathrm{r}(t) = (\mathbf{proc}(t) \ldots \mathbf{end\ proc})]$$

```
> polarplot([rhs(Eq51(t)[3]), rhs(Eq51(t)[2]), t=-Pi..Pi],
> scaling=constrained);
```

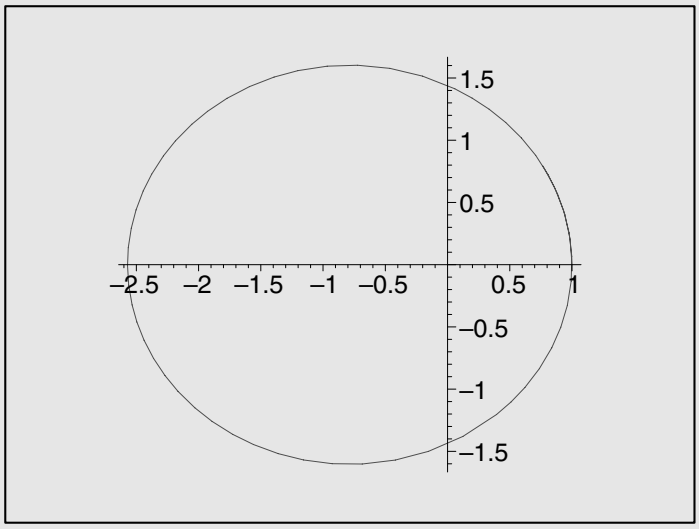



```
> Eq64 := D(phi)(0) = 1.2:
> En := eval(T + V, {r(t)=rhs(Eq41), diff(r(t),t)=rhs(Eq42),
> diff(phi(t),t)=rhs(Eq64)}):
> l := eval(lhs(Eq14), {r(t)=rhs(Eq41),
> diff(phi(t),t)=rhs(Eq64)}):
> epsilon := sqrt(1 + 2*En*l^2/(m*(G*M*m)^2));
```

$$\varepsilon := 0.4400000000$$

```
> ini2 := Eq41, Eq42, Eq43:
> Eq71:=dsolve({Eq31, Eq32, ini2}, {r(t), phi(t)}, numeric,
> output=listprocedure):
```

```
> polarplot([rhs(Eq71(t)[3]), rhs(Eq71(t)[2]), t=0..5*Pi],
> scaling=constrained);
```




```
> Eq84 := D(phi)(0) = 1.5:

> En := eval(T + V, {r(t)=rhs(Eq41), diff(r(t),t)=rhs(Eq42),
> diff(phi(t),t)=rhs(Eq84)}):

> l := eval(lhs(Eq14), {r(t)=rhs(Eq41),
> diff(phi(t),t)=rhs(Eq84)}):

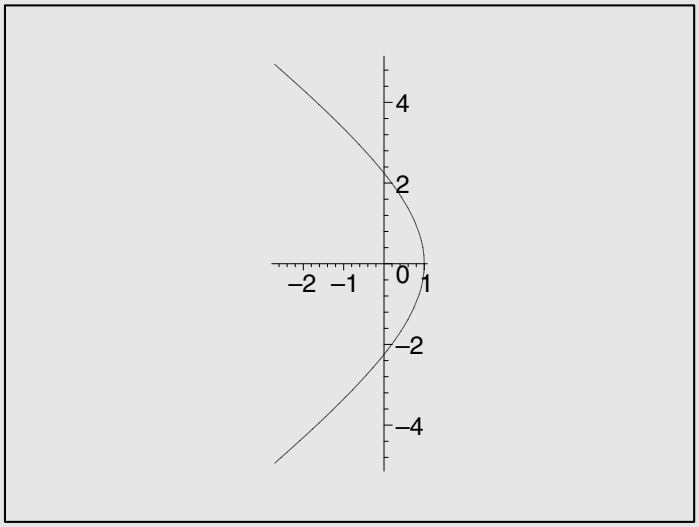
> epsilon := sqrt(1 + 2*En*l^2/(m*(G*M*m)^2));
```

$$\varepsilon := 1.250000000$$

```
> ini2 := Eq41, Eq42, Eq43:

> Eq91:=dsolve({Eq31, Eq32, ini2}, {r(t), phi(t)}, numeric,
> output=listprocedure):
```

```
> polarplot([rhs(Eq91(t)[3]), rhs(Eq91(t)[2]), t=-2*Pi..2*Pi],
> scaling=constrained);
```




```
> Eq104 := D(phi)(0) = sqrt(2):

> En := eval(T + V, {r(t)=rhs(Eq41), diff(r(t),t)=rhs(Eq42),
> diff(phi(t),t)=rhs(Eq104)}):

> l := eval(lhs(Eq14), {r(t)=rhs(Eq41),
> diff(phi(t),t)=rhs(Eq104)}):

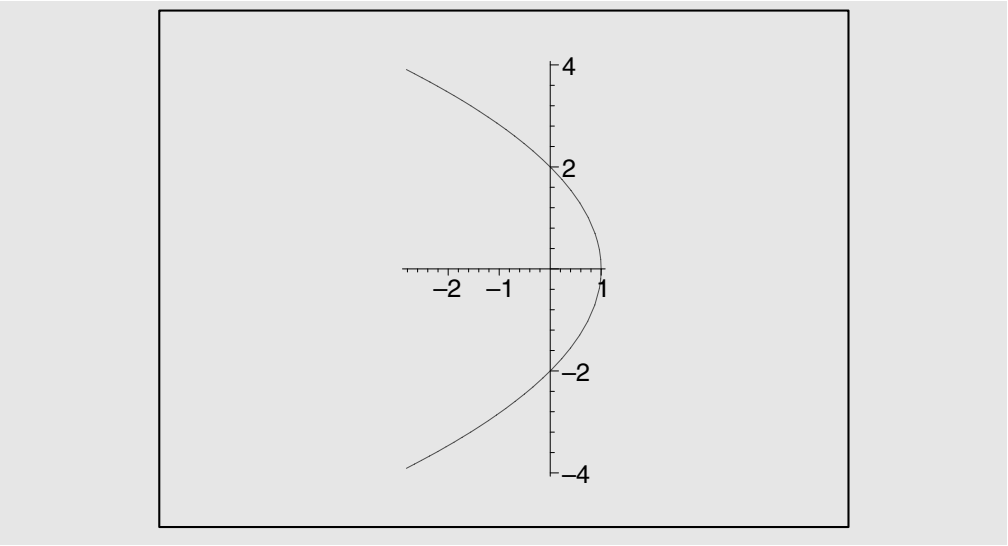
> epsilon := sqrt(1 + 2*En*l^2/(m*(G*M*m)^2));
```

$$\varepsilon := 1$$

```
> ini2 := Eq41, Eq42, Eq43:

> Eq111:=dsolve({Eq31, Eq32, ini2}, {r(t), phi(t)}, numeric,
> output=listprocedure):

> polarplot([rhs(Eq111(t)[3]), rhs(Eq111(t)[2]), t=-2*Pi..2*Pi],
> scaling=constrained);
```



The Kepler problem admits an analytic solution, which is discussed in standard textbooks on classical mechanics.[1] An alternative way to solve the Kepler problem is to use the properties of conservation of energy and of angular momentum. The former condition gives

$$E = \text{constant} = T + V = \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\phi}^2 - \frac{GMm}{r}, \tag{4.24}$$

and the latter gives

$$l = \text{constant} = mr^2\dot{\phi}, \tag{4.25}$$

both first-order differential equations. Using

$$\frac{1}{2}mr^2\dot{\phi}^2 = \frac{l^2}{2mr^2},$$

we eliminate $\dot{\phi}$ so that equation (4.24) becomes a first-order differential equation. To solve this equation, we obtain a relation between r and t as

$$\dot{r} = \frac{dr}{dt} = \sqrt{\frac{2}{m}\left(E + \frac{GMm}{r}\right) - \frac{l^2}{m^2r^2}}, \quad dt = \frac{dr}{\sqrt{\frac{2}{m}\left(E + \frac{GMm}{r}\right) - \frac{l^2}{m^2r^2}}}, \tag{4.26}$$

and integration over dt yields t as a function of r.

To find the trajectory, we rearrange equation (4.25) to

$$dt = \frac{mr^2}{l}d\phi, \tag{4.27}$$

[1] Goldstein et al. 2002, p. 92ff.

and eliminate time from the previous equation. We obtain $\phi(r)$ on evaluating an integral

$$\phi = \int \frac{l}{r^2\sqrt{2m\left(E + \frac{GMm}{r}\right) - \frac{l^2}{r^2}}}\, dr. \tag{4.28}$$

Maple evaluates this integral exactly:

$$\phi = \tan^{-1} \frac{m^2 rGM - l^2}{l\sqrt{2mr^2E + 2m^2rGM - l^2}} + \text{constant}. \tag{4.29}$$

Worksheet 4.4

```
> assume(l>0, r>0):
> Epr1 := l/(r^2*sqrt(2*m*(En + G*M*m/r) - l^2/r^2));
```

$$Epr1 := \frac{l}{r^2\sqrt{2\,m\,(En + \frac{G\,M\,m}{r}) - \frac{l^2}{r^2}}}$$

```
> Epr2 := int(Epr1, r):
> Epr3 := simplify(Epr2);
```

$$Epr3 := \arctan(\frac{-l^2 + m^2\,r\,G\,M}{l\,\sqrt{2\,m\,r^2\,En + 2\,m^2\,r\,G\,M - l^2}})$$

Although we might use equation (4.29) to depict the trajectory, we leave it as an exercise for the reader to make trigonometric rearrangement of the Maple output so as to express it in a more conventional format, namely an equation of a conic section in polar coordinates,

$$r = \frac{l^2}{m(GMm)} \frac{1}{1 + \epsilon\cos\phi}, \tag{4.30a}$$

where ϵ represents the eccentricity,

$$\epsilon = \sqrt{1 + \frac{2l^2E}{m(GMm)^2}}. \tag{4.30b}$$

From our numerical experiments, we observe that the shape of the orbit depends on ϵ according to the following conditions.

$\epsilon = 0,$	$E = -\frac{1}{2}\frac{m(GMm)^2}{l^2},$	circle
$\epsilon < 1,$	$E < 0,$	ellipse
$\epsilon > 1,$	$E > 0,$	hyperbola
$\epsilon = 1,$	$E = 0,$	parabola.

4.3.2 Correction Terms

The planet Mercury is observed to move in an elliptical orbit, but this orbit does not quite close upon itself. The ellipse rotates, and the perihelion – the point on its orbit that is nearest the Sun – advances; this phenomenon is called precession. In our consideration of planetary motion in the preceding section, our concern was a system of only two bodies, governed purely by a potential of form r^{-1}. Any departure from this idealized potential produces precession, which we discuss here.

Although the Sun is the dominant source of gravity in the solar system, other planets also exert an influence on Mercury. We can write the correction terms as expansion of r^{-1} to various powers. For example, if we add a r^{-2} term to the potential, the differential equation remains exactly solvable, and precession results therefrom. The solution is listed in an exercise at the end of the chapter.

Furthermore, the inverse-square law of force applies to two spherical bodies. The Sun is not perfectly spherical: because the Sun rotates with a period of about 25 days, which causes a solar equatorial bulge. This oblate Sun can be considered to have a quadrupole moment, for which the potential energy is proportional to r^{-3}. According to our numerical treatment of the Kepler problem, we readily proceed to include this contribution to potential energy; with such a term in our Lagrangian we also obtain a precessing orbit.

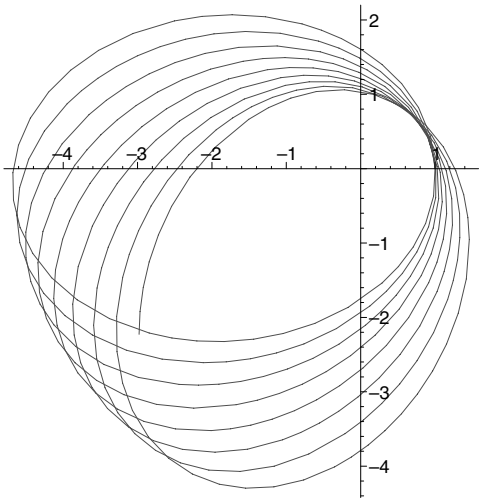


Figure 4.2: Precession induced by a quadrupole term.

Example 4.1 Observe the behavior of the orbit under the potential

$$V = -\frac{GMm}{r} - k'\frac{1}{r^3}. \tag{4.31}$$

Solution In this example, we suppose $k' = 2 \times 10^{-2}$, and again set G, M and m to unity. With these initial conditions,

$$r_0 = 1, \quad \dot{r}_0 = 0, \quad \phi_0 = 0, \quad \dot{\phi}_0 = 1.3,$$

we evaluate energy and angular momentum as

$$E = -0.175, \quad l = 1.3.$$

With a slight modification of the worksheet in the preceding section, we obtain a plot shown in Figure 4.2. One should experiment with other numerical values.

To take into account of any additional contributions of forces from other bodies, we simply modify the function for potential energy according to the physical situation. Approximate methods, such as perturbation theory explained in advanced courses on mechanics, are conventionally employed to take these effects into account, but in using Maple to solve a differential equation numerically we can directly observe the effects that provide us with physical insight.

After all possible corrections from Newtonian mechanics are exhausted, there remains a small discrepancy in the precession of Mercury's orbit; an explanation has to await general relativity. To calculate the precession of Mercury, we can add a correction term to the potential energy, of a form also proportional to r^{-3}, to take account of the general relativistic effect within the framework of Newtonian mechanics. For planetary motion in a strong gravitational field, such as near a neutron star or a black hole, we must apply general relativity, which is the subject of Chapter 18. The principle of least action is still applicable: we merely use a corresponding Lagrangian in general relativity.

4.4 Motion of a Symmetric Top

We next consider a symmetric top under the influence of gravity with one point fixed, discussed at length in many books on advanced mechanics.[2] It is convenient to specify the configuration of the top by three Euler angles. Let $OXYZ$ be a Cartesian coordinate system fixed in space, and let $Oxyz$ be rectangular axes fixed relatively to the body and moving with it, such that θ specifies the inclination of axis z from the vertical, ϕ measures the azimuth of the top about the vertical direction, and ψ is the angle of rotation of the top about its own z axis; see Figure 4.3. Note that the definition of the Euler angles varies widely; our notation conforms to that of Goldstein et al. The transformation between the two sets of axes $OXYZ$ and $Oxyz$ is

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = A \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} \tag{4.32a}$$

[2] Goldstein et al. 2002, p. 209ff.

where

$$A = \begin{pmatrix} \cos\psi\cos\phi - \cos\theta\sin\phi\sin\psi & \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\psi\sin\theta \\ -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & -\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi & \cos\psi\sin\theta \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{pmatrix}. \tag{4.32b}$$

The inverse transformation from body coordinates $\mathbf{x}$ to space coordinates $\mathbf{X}$ is $\mathbf{X} = A^{-1}\mathbf{x}$, where A^{-1} is equal to the transpose A^T of A. The components of angular velocity with respect to the body axes in terms of Euler angles are

$$\begin{aligned} \omega_1 &= \dot{\phi}\sin\theta\sin\psi + \dot{\theta}\cos\psi \\ \omega_2 &= \dot{\phi}\sin\theta\cos\psi - \dot{\theta}\sin\psi \\ \omega_3 &= \dot{\phi}\cos\theta + \dot{\psi}. \end{aligned} \tag{4.33}$$

Let the axis of symmetry be taken as z fixed in the top; the moment of inertia is I_3 about this axis, and symmetry requires $I_1 = I_2$. The kinetic energy is

$$T = \frac{1}{2}I_1(\omega_1^2 + \omega_2^2) + \frac{1}{2}I_3\omega_3^2, \tag{4.34}$$

or in terms of Euler angles

$$T = \frac{I_1}{2}(\dot{\theta}^2 + \dot{\phi}^2\sin^2\theta) + \frac{I_3}{2}(\dot{\psi} + \dot{\phi}\cos\theta)^2. \tag{4.35}$$

The potential energy is

$$V = mgl\cos\theta. \tag{4.36}$$

The Lagrangian is

$$L = \frac{I_1}{2}(\dot{\theta}^2 + \dot{\phi}^2\sin^2\theta) + \frac{I_3}{2}(\dot{\psi} + \dot{\phi}\cos\theta)^2 - mgl\cos\theta. \tag{4.37}$$

Because ϕ and ψ do not appear explicitly in the Lagrangian, the corresponding generalized momenta are constant in time. Applying the Euler–Lagrange equations, we obtain

$$p_\psi = \frac{\partial L}{\partial\dot{\psi}} = I_3(\dot{\psi} + \dot{\phi}\cos\theta) \equiv M_z, \tag{4.38}$$

$$p_\phi = \frac{\partial L}{\partial\dot{\phi}} = I_3(\dot{\psi} + \dot{\phi}\cos\theta)\cos\theta + I_1\dot{\phi}\sin^2\theta \equiv M_{z'}, \tag{4.39}$$

and

$$I_1\ddot{\theta} - (I_1 - I_3)\dot{\phi}^2\sin\theta\cos\theta + I_3\dot{\phi}\dot{\psi}\sin\theta - mgl\sin\theta = 0. \tag{4.40}$$

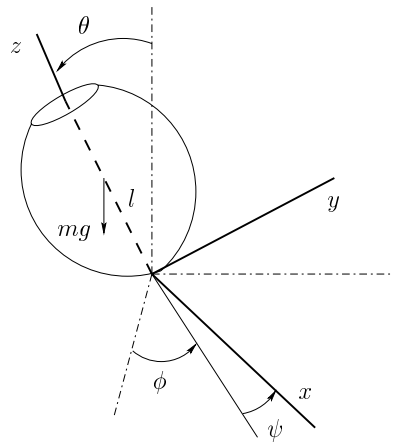


Figure 4.3: Euler angles to specify the orientation of a symmetric top.

With the initial conditions θ_0, $\dot{\theta}_0$, ϕ_0, $\dot{\phi}_0$, ψ_0 and $\dot{\psi}_0$, we can solve the above differential equations.

Although it is unnecessary for computational purposes, we rearrange the above three equations so that a reader can compare them with those in most textbooks. For $\dot{\phi}$ and $\dot{\psi}$ in terms of θ, we have

$$\dot{\phi} = \frac{M_{z'} - M_z \cos\theta}{I_1 \sin^2\theta}, \tag{4.41}$$

and

$$\dot{\psi} = \frac{M_z}{I_3} - \frac{M_{z'} - M_z \cos\theta}{I_1 \sin^2\theta} \cos\theta. \tag{4.42}$$

We hence derive an equation involving only θ as variable,

$$I_1\ddot{\theta} - \frac{(M_{z'} - M_z \cos\theta)^2 \cos\theta}{I_1 \sin^3\theta} + \frac{(M_{z'} - M_z \cos\theta) M_z}{I_1 \sin\theta} - mgl \sin\theta = 0. \tag{4.43}$$

As M_z and $M_{z'}$ are constant, we can evaluate them from the provided initial conditions:

$$M_z = I_3(\dot{\psi}_0 + \dot{\phi}_0 \cos\theta_0), \tag{4.44}$$

and

$$M_{z'} = I_3(\dot{\psi}_0 + \dot{\phi}_0 \cos\theta_0)\cos\theta_0 + I_1 \dot{\phi}_0 \sin^2\theta_0. \tag{4.45}$$

Having solved the θ equation, we can integrate the ϕ and ψ equations. We consider a numerical example.

Example 4.2 A top constructed from a heavy circular disk of mass $m = 100.0$ g and radius 2.0 cm is mounted at the center of a thin rod of length 4.0 cm; see Figure 4.4. Suppose that we set the top to spin at 35 rev s^{-1}, and place it at an angle $\theta_0 = 60^\circ$ from the vertical. We assume $\dot{\theta}_0 = 0$, and discuss three situations: (a) $\dot{\phi}_0 = -5$ rad s^{-1} ; (b) $\dot{\phi}_0 = 0$ rad s^{-1}; (c) $\dot{\phi}_0 = 1$ rad s^{-1}.

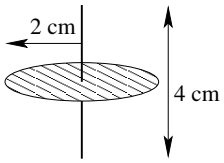


Figure 4.4: A symmetric top of mass 100.0 g.

Solution According to the figure, $l = 0.02$ m and $R = 0.02$ m. We calculate the moment of inertia: for I_1,

$$I_1 = \frac{1}{4}mR^2 + ml^2,$$

and for I_2,

$$I_2 = \frac{1}{2}mR^2.$$

The top was set to spin at 35 rev s^{-1} initially; therefore

$$\dot{\psi}_0 = (2\pi)(35) = 219.9 \text{ (rad s}^{-1}\text{)}.$$

Worksheet 4.5 This worksheet is similar to several preceding worksheets: after defining kinetic and potential energies, we make substitutions to obtain the equations of motion; `Eq14` concerns the ψ coordinate with a constant `Mz` (for M_z), `Eq24` for ϕ with a constant `Mz1` (for $M_{z'}$), and `Eq36` for θ. We rearrange these equations with the `isolate` command. We introduce the `spacecurve` command from the `plots` package to produce a curve for the locus of the figure axis.

```
> T := I1/2*(diff(theta(t),t)^2 + diff(phi(t),t)^2*sin(theta(t))^2)
> + I3/2*(diff(psi(t),t) + diff(phi(t),t)*cos(theta(t)))^2;
```

$$T := \frac{1}{2}\,I1\,((\tfrac{d}{dt}\,\theta(t))^2 + (\tfrac{d}{dt}\,\phi(t))^2\sin(\theta(t))^2) + \frac{1}{2}\,I3\,((\tfrac{d}{dt}\,\psi(t)) + (\tfrac{d}{dt}\,\phi(t))\cos(\theta(t)))^2$$

```
> V := m*g*l*cos(theta(t));
```

$$V := m\,g\,l\cos(\theta(t))$$

```
> L := T - V;
```

$$L := \frac{1}{2}\,I1\,((\tfrac{d}{dt}\,\theta(t))^2 + (\tfrac{d}{dt}\,\phi(t))^2\sin(\theta(t))^2) + \frac{1}{2}\,I3\,((\tfrac{d}{dt}\,\psi(t)) + (\tfrac{d}{dt}\,\phi(t))\cos(\theta(t)))^2 - m\,g\,l\cos(\theta(t))$$

```
> L1 := subs({phi(t)=var1, theta(t)=var2, psi(t)=var3,
> diff(phi(t),t)=var4, diff(theta(t),t)=var5,
diff(psi(t),t)=var6},L):
> Epr11 := diff(L1,var6):
> Epr13 := subs({var1=phi(t), var2=theta(t), var3=psi(t),
> var4=diff(phi(t),t), var5=diff(theta(t),t), var6=diff(psi(t),t)},
> Epr11):
> Eq14 := Epr13 = Mz;
```

$$Eq14 := I3\,((\tfrac{d}{dt}\,\psi(t)) + (\tfrac{d}{dt}\,\phi(t))\cos(\theta(t))) = Mz$$

```
> Epr21 := diff(L1,var4):
> Epr23 := subs({var1=phi(t), var2=theta(t), var3=psi(t),
> var4=diff(phi(t),t), var5=diff(theta(t),t), var6=diff(psi(t),t)},
> Epr21):
> Eq24 := Epr23 = Mz1;
```

$$Eq24 := I1\,(\tfrac{d}{dt}\,\phi(t))\sin(\theta(t))^2 + I3\,((\tfrac{d}{dt}\,\psi(t)) + (\tfrac{d}{dt}\,\phi(t))\cos(\theta(t)))\cos(\theta(t)) = Mz1$$

```
> Epr31 := diff(L1,var5):
> Epr32 := diff(L1,var2):
> Epr33 := subs({var1=phi(t), var2=theta(t), var3=psi(t),
> var4=diff(phi(t),t), var5=diff(theta(t),t), var6=diff(psi(t),t)},
> Epr31):
> Epr34 := subs({var1=phi(t), var2=theta(t), var3=psi(t),
> var4=diff(phi(t),t), var5=diff(theta(t),t), var6=diff(psi(t),t)},
> Epr32):
> Epr35 := diff(Epr33,t):
> Eq36 := Epr35 - Epr34 = 0;
```

$$Eq36 := I1\,(\tfrac{d^2}{dt^2}\,\theta(t)) - I1\,(\tfrac{d}{dt}\,\phi(t))^2\sin(\theta(t))\cos(\theta(t))$$
$$+ I3\,((\tfrac{d}{dt}\,\psi(t)) + (\tfrac{d}{dt}\,\phi(t))\cos(\theta(t)))\,(\tfrac{d}{dt}\,\phi(t))\sin(\theta(t)) - m\,g\,l\sin(\theta(t)) = 0$$

```
> Eq51 := isolate(Eq14, diff(psi(t),t)):
> Eq52 := isolate(Eq24, diff(psi(t),t)):
> Eq53 := rhs(Eq51) = rhs(Eq52);
```

$$Eq53 := \frac{Mz}{I3} - (\tfrac{d}{dt}\,\phi(t))\cos(\theta(t))$$
$$= \frac{Mz1 - I1\,(\tfrac{d}{dt}\,\phi(t))\sin(\theta(t))^2}{I3\cos(\theta(t))} - (\tfrac{d}{dt}\,\phi(t))\cos(\theta(t))$$

```
> Eq54 := isolate(Eq53, diff(phi(t),t));
```

$$Eq54 := \frac{d}{dt}\,\phi(t) = -\frac{Mz\cos(\theta(t)) - Mz1}{I1\sin(\theta(t))^2}$$

```
> Eq55 := eval(Eq51, Eq54);
```

$$Eq55 := \frac{d}{dt}\,\psi(t) = \frac{Mz}{I3} + \frac{(Mz\cos(\theta(t)) - Mz1)\cos(\theta(t))}{I1\sin(\theta(t))^2}$$

```
> Eq61 := eval(Eq36, {Eq54, Eq55});
```

$$Eq61 := I1\,(\frac{d^2}{dt^2}\,\theta(t)) - \frac{(Mz\cos(\theta(t)) - Mz1)^2\cos(\theta(t))}{I1\sin(\theta(t))^3}$$
$$-\frac{Mz\,(Mz\cos(\theta(t)) - Mz1)}{I1\sin(\theta(t))} - m\,g\,l\sin(\theta(t)) = 0$$

```
> with(plots):
Warning, the name changecoords has been redefined
> g:=9.8; m:=0.1; l:=0.02; R:=0.02;
```

$$g := 9.8$$
$$m := 0.1$$
$$l := 0.02$$
$$R := 0.02$$

```
> I1 := m*l^2;
```

$$I1 := 0.00004$$

```
> I3 := 1/2*m*R^2;
```

$$I3 := 0.00002000000000$$

```
> Eq70 := psi(0) = 0;
```

$$Eq70 := \psi(0) = 0$$

```
> Eq71 := D(psi)(0) = evalf(35*2*Pi);
```

$$Eq71 := \mathrm{D}(\psi)(0) = 219.9114858$$

```
> Eq72 := phi(0) = 0;
```

$$Eq72 := \phi(0) = 0$$

```
> Eq73 := D(phi)(0) = -5;          #try different values
```

$$Eq73 := \mathrm{D}(\phi)(0) = -5$$

```
> Eq74 := theta(0) = evalf(Pi/3);
```

$$Eq74 := \theta(0) = 1.047197551$$

```
> Eq75 := D(theta)(0) = 0;
```

$$Eq75 := \mathrm{D}(\theta)(0) = 0$$

```
> Mz := eval(lhs(Eq14), {diff(psi(t),t) = rhs(Eq71), diff(phi(t),t)
> = rhs(Eq73), theta(t)=rhs(Eq74)});
```

$$Mz := 0.004348229716$$

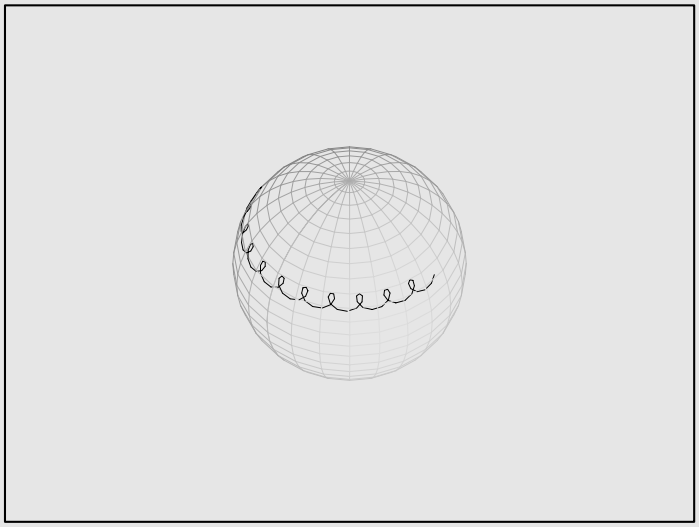
```
> Mz1 := eval(lhs(Eq24), {diff(psi(t),t) = rhs(Eq71),diff(phi(t),t)
> = rhs(Eq73), theta(t)=rhs(Eq74)});
```

$$Mz1 := 0.002024114858$$

```
> Eq91 := dsolve({Eq54, Eq55, Eq61, Eq70, Eq72, Eq74, Eq75},
> {theta(t), phi(t), psi(t)}, numeric);
```

$$Eq91 := \mathbf{proc}(x_rkf45) \ldots \mathbf{end\ proc}$$

```
> p1 := odeplot(Eq91, [l*sin(theta(t))*sin(phi(t)),
> -l*sin(theta(t))*cos(phi(t)), l*cos(theta(t))], 0..0.7,
> numpoints=100, thickness=2, color=black):
> p2 := sphereplot(l, theta=0..2*Pi, phi=0..Pi, style=hidden):
> display([p1,p2], scaling=constrained);
```



```
> Eq73 := D(phi)(0) = 0;
```

$$Eq73 := \mathrm{D}(\phi)(0) = 0$$

```
> Mz;
```

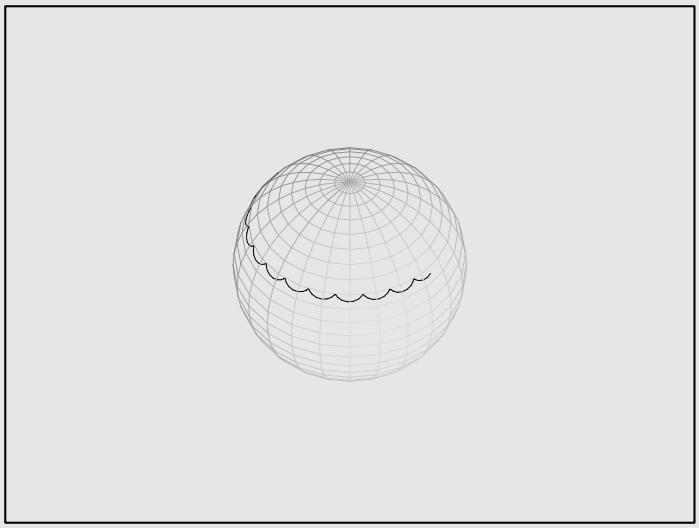
$$0.004348229716$$

```
> Mz1 := eval(lhs(Eq24), {diff(psi(t),t) = rhs(Eq71),
diff(phi(t),t) =
> rhs(Eq73), theta(t)=rhs(Eq74)});
```

$$Mz1 := 0.002199114858$$

```
> Eq91 := dsolve({Eq54, Eq55, Eq61, Eq70, Eq72, Eq74, Eq75},
> {theta(t), phi(t), psi(t)}, numeric, output=listprocedure):
```

```
> p3 := odeplot(Eq91, [l*sin(theta(t))*sin(phi(t)),
> -l*sin(theta(t))*cos(phi(t)), l*cos(theta(t))], 0..0.7,
> numpoints=100, thickness=2, color=black):
> display([p3, p2], scaling=constrained);
```



```
> Eq73 := D(phi)(0) = 1;
```

$$Eq73 := \mathrm{D}(\phi)(0) = 1$$

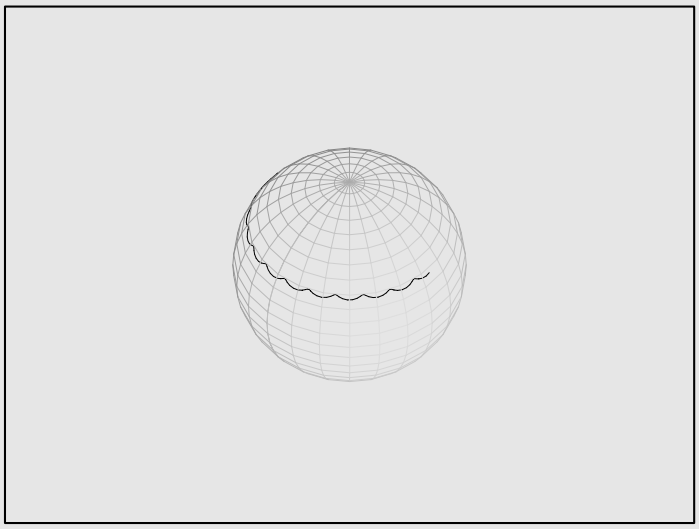
```
> Mz;
```

$$0.004348229716$$

```
> Mz1 := eval(lhs(Eq24), {diff(psi(t),t) = rhs(Eq71),diff(phi(t),t)
> = rhs(Eq73), theta(t)=rhs(Eq74)});
```

$$Mz1 := 0.002234114858$$

```
> Eq91 := dsolve({Eq54, Eq55, Eq61, Eq70, Eq72, Eq74, Eq75},
> {theta(t), phi(t), psi(t)}, numeric, output=listprocedure):
> p4 := odeplot(Eq91, [l*sin(theta(t))*sin(phi(t)),
> -l*sin(theta(t))*cos(phi(t)), l*cos(theta(t))], 0..0.7,
> numpoints=100, thickness=2, color=black):
> display([p4, p2], scaling=constrained);
```



We depict the motion of the top by tracing a curve of the intersection of the figure axis with the surface of a sphere of unit radius about the fixed point; this curve is called the locus of the figure axis. The motion in the ϕ direction is known as precession, and in the θ direction is known as nutation. In our numerical examples, we observe three possible shapes for the locus of the figure axis. If $\dot{\phi}_0$ is negative, it exhibits loops; if $\dot{\phi}_0 = 0$, the locus has cusps; and if $\dot{\phi}_0$ is positive, ϕ increases secularly in one direction.

4.5 Nonlinear Oscillation and Chaos

We have discussed linear oscillatory systems extensively in Chapter 2. For most systems, however, the equation of motion is linear for only a limited range of conditions. When the amplitude of oscillations is large, one needs to include higher terms of the potential energy:

$$V = \frac{1}{2}m\omega_0^2 x^2 + \frac{1}{3}m\delta x^3 + \frac{1}{4}m\beta x^4 + \ldots.$$

Suppose there is no friction, the equation of motion for this system is

$$\ddot{x} + \omega_0^2 x + \delta x^2 + \beta x^3 + \ldots = 0.$$

In most situations this equation admits no analytic solution; one might find a textbook presenting the perturbation theory by expressing the solution as a series of successive approximations: $x = x^{(1)} + x^{(2)} + x^{(3)} + \ldots$, where the dominant term is

$$x^{(1)} = A\cos\omega_f t, \tag{4.46}$$

with the value of the fundamental natural frequency ω_f expressed as $\omega_f = \omega_0 + \omega^{(1)} + \omega^{(2)} + \ldots$. An important property pertaining to a nonlinear system is that the solution contains terms of the combination of frequencies ($2\omega_f$ in $x^{(2)}$, $3\omega_f$ in $x^{(3)}$, etc.), and the fundamental natural frequency ω_f deviates from ω_0. We use the following example to illustrate this point.

A common model for anharmonic oscillator has the Lagrangian in the form

$$L = \frac{1}{2}m\dot{x}^2 - V, \quad V = \frac{1}{2}m\alpha x^2 + \frac{1}{4}m\beta x^4. \tag{4.47}$$

(We use α for ω_0^2.) The equation of motion for this system is

$$\ddot{x} + \alpha x + \beta x^3 = 0. \tag{4.48}$$

This equation is actually exactly solvable. Rather than solving a second-order differential equation, with the aid of conservation of energy we express the sum of potential and kinetic energies as

$$\frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\alpha x^2 + \frac{1}{4}m\beta x^4 = \frac{1}{2}m\alpha A^2 + \frac{1}{4}m\beta A^4, \tag{4.49}$$

where A is the maximum displacement. (That is $\dot{x} = 0$ when $x = A$.) The conservative quantity yields a first-order differential equation:

$$\frac{dx}{dt} = \sqrt{2}\sqrt{\frac{1}{2}\alpha A^2 + \frac{1}{4}\beta A^4 - \frac{1}{2}\alpha x^2 - \frac{1}{4}\beta x^4},$$

and is solved as

$$t = \sqrt{\frac{1}{2}}\int_0^x \frac{dx'}{\sqrt{\frac{1}{2}\alpha A^2 + \frac{1}{4}\beta A^4 - \frac{1}{2}\alpha x'^2 - \frac{1}{4}\beta x'^4}}. \tag{4.50}$$

This solution is an elliptic integral, which is not particularly relevant to our discussion; we are interested in the oscillating frequency. The time to move from $x = A$ to $x = 0$ corresponds to a quarter period:

$$\frac{\tau_0}{4} = \sqrt{\frac{1}{2}}\int_0^A \frac{dx}{\sqrt{\frac{1}{2}\alpha A^2 + \frac{1}{4}\beta A^4 - \frac{1}{2}\alpha x^2 - \frac{1}{4}\beta x^4}}. \tag{4.51}$$

Although the fundamental natural frequency, $2\pi/\tau_0$, can be written exactly as an elliptic integral (see the worksheet below) we approximate it as a linear function in β to make its dependence on α, β and A explicit:

$$\omega_f = \frac{2\pi}{\tau_0} \cong \sqrt{\alpha} + \frac{3\beta}{8\sqrt{\alpha}}A^2. \tag{4.52}$$

We see that nonlinearity of the oscillations has an amplitude dependence of the fundamental natural frequency; the correction term is proportional to the squared amplitude of the oscillations.

Worksheet 4.6 Maple transforms equation (4.51) into an elliptic integral; we then use the `taylor` command to expand the elliptic integral and retain only β to the first power.

```
> assume(A>0, alpha>0, beta>0):
> tau0 := 4/sqrt(2)*int(1/sqrt(1/2*alpha*A^2 + 1/4*beta*A^4 -
> 1/2*alpha*x^2 - 1/4*beta*x^4), x=0..A);
```

$$\tau 0 := \frac{4\,\mathrm{EllipticK}\left(\dfrac{\sqrt{2}\,A\sqrt{\dfrac{\beta}{\beta\,A^2+\alpha}}}{2}\right)}{\sqrt{\dfrac{\beta\,A^2+\alpha}{\beta}}\,\sqrt{\beta}}$$

```
> taylor(2*Pi/tau0, beta, 2);
```

$$\sqrt{\alpha} + \frac{3\,A^2}{8\sqrt{\alpha}}\,\beta + \mathrm{O}(\beta^2)$$

Now we consider forced nonlinear oscillations, which Maple can conveniently solve using the numerical method. By adding an external periodic force of frequency ω to equation (4.48) and including the damping force $b\dot{x}$, we have

$$\ddot{x} + \frac{b}{m}\dot{x} + \alpha x + \beta x^3 = \frac{F_0}{m}\cos(\omega t). \tag{4.53}$$

This equation is known as the Duffing equation. It is worthwhile to compare a forced nonlinear oscillator with a linear one, which we have analytically solved in Section 2.3:

$$\ddot{x} + \frac{b}{m}\dot{x} + \omega_0^2 x = \frac{F_0}{m}\cos(\omega t). \tag{4.54}$$

The solution to the linear equation contains a transient part and a steady-state part; the latter is interpreted as the force response. If the driven frequency ω is set at the natural frequency ω_0, the amplitude of the steady-state solution becomes very large, a phenomenon called resonance.

Under certain conditions, the system with an anharmonic term oscillates with a nearly constant amplitude, but it exhibits new properties which are absent in a linear system.

Worksheet 4.7 We enter the differential equation. After providing all the numerical values of parameters and initial conditions, we solve the equation numerically and plot the force response. The time in the plot starts at 60 s to exclude the transient effect.

```
> Eq1 := diff(x(t),t$2) + b/m*diff(x(t),t)
> + alpha*x(t) + beta*x(t)^3 = F0/m*cos(omega*t);
```

$$Eq1 := (\tfrac{d^2}{dt^2}\,\mathrm{x}(t)) + \frac{b\,(\frac{d}{dt}\,\mathrm{x}(t))}{m} + \alpha\,\mathrm{x}(t) + \beta\,\mathrm{x}(t)^3 = \frac{F0\cos(\omega\,t)}{m}$$

```
> m := 1; b := .2; beta := 1; alpha := 1; F0 := 3; omega := 3;
```

$$m := 1$$
$$b := 0.2$$
$$\beta := 1$$
$$\alpha := 1$$
$$F0 := 3$$
$$\omega := 3$$

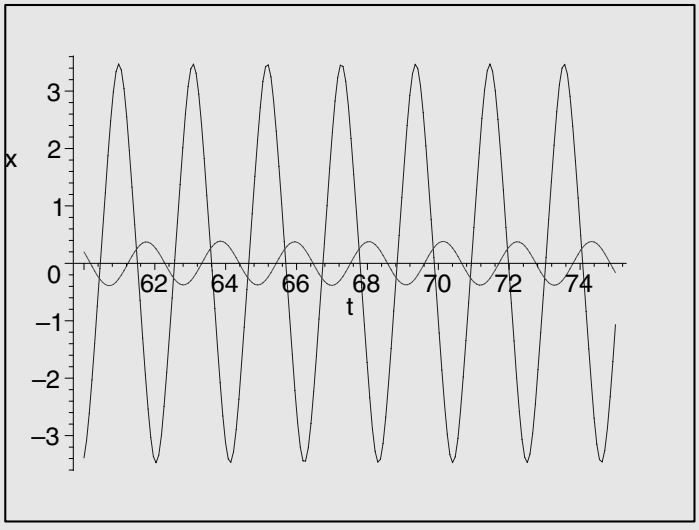
```
> Soln1 := dsolve({Eq1, x(0)=2, D(x)(0)=0}, x(t), numeric);
```

$$Soln1 := \mathbf{proc}(x_rkf45)\ \ldots\ \mathbf{end\ proc}$$

```
> Soln2 := dsolve({Eq1, x(0)=3.1, D(x)(0)=0}, x(t), numeric);
```

$$Soln2 := \mathbf{proc}(x_rkf45)\ \ldots\ \mathbf{end\ proc}$$

```
> with(plots):
Warning, the name changecoords has been redefined
> p1 := odeplot(Soln1, [t, x(t)], 60..75, numpoints=200):
> p2 := odeplot(Soln2, [t, x(t)], 60..75, numpoints=200,
> color=blue):
> display([p1, p2]);
```



From the graph, we observe that a given driven frequency could result in two different amplitudes of oscillation. To understand this property, we start with the formula of the response curve of a linear oscillator (equation (2.17)):

$$A = \frac{F_0}{\sqrt{m^2(\omega_0^2 - \omega^2)^2 + b^2\omega^2}} \tag{4.55}$$

For a nonlinear oscillator, ω_0 is replaced by ω_f, see equation (4.52), which contains an amplitude-dependent correction. The square of the fundamental frequency is approximated as

$$\omega_f^2 = \left(\sqrt{\alpha} + \frac{3\beta}{8\sqrt{\alpha}}A^2\right)^2 \cong \alpha + \frac{3}{4}\beta A^2,$$

Replacing ω_0^2 by $\alpha + \frac{3}{4}\beta A^2$ in equation(4.55), we obtain the lowest-order approximation of the response curve for a nonlinear oscillator

$$F_0^2 = A^2\left[m^2\left(\alpha + \frac{3\beta}{4}A^2 - \omega^2\right)^2 + b^2\omega^2\right]. \tag{4.56}$$

Worksheet 4.8 We use the `implicitplot` command to plot the response curve.

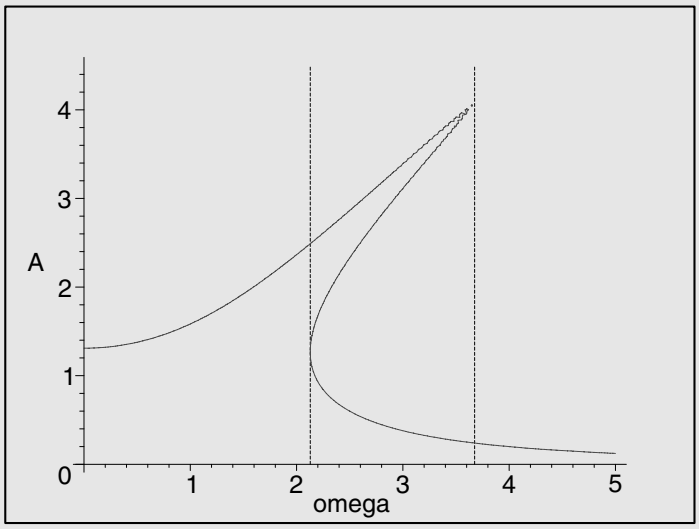
```
> Eq1 := A^2*(m^2*(alpha-omega^2+3*beta/4*A^2)^2 + b^2*omega^2) =
> F0^2;
```

$$Eq1 := A^2\left(m^2\left(\alpha - \omega^2 + \frac{3\,\beta\,A^2}{4}\right)^2 + b^2\,\omega^2\right) = F0^2$$

```
> m := 1; b := .2; beta := 1; alpha := 1; F0 := 3;
```

$$m := 1$$
$$b := 0.2$$
$$\beta := 1$$
$$\alpha := 1$$
$$F0 := 3$$

```
> with(plots):
Warning, the name changecoords has been redefined
> implicitplot(Eq1, omega=0..5, A=0..5, numpoints=10000);
```



The response curve display a tilt (comparing with the response curve in Section 2.3); to be more precise, it is a cubic equation in A^2. From the graph it is clear that there exists a range of frequencies (from about $\omega \approx 2.1$ to $\omega \approx 3.7$ in the above worksheet) in which A can be multivalued. The physical interpretation is that in this range of frequencies different amplitudes of oscillations are possible. It can be proved that the middle branch corresponds to unstable oscillations. At $\omega = 3$, the upper root is about $A = 3.4$, and the lower one is about $A = 0.4$; these values are consistent with the amplitude from numerical solution in the preceding worksheet. One should try different driven frequencies ω and initial conditions to verify the response curve. Physically, if one starts at a low frequency and gradually increases the frequency, the amplitude will rise following the curve up to a maximum at about $\omega \approx 3.7$, then a slight increase will cause the amplitude to "jump down" to the lower branch. On the other hand, if one starts at a high frequency and gradually decreases the frequency, the amplitude will "jump up" to the upper branch at about $\omega \approx 2.1$. This phenomenon is know as *hysteresis*, meaning that the force response depends on how one scans the frequencies.

To conclude this section, we demonstrate a system that oscillates rather chaotically under certain conditions. We use an equation

$$\ddot{x} + 0.5\dot{x} - x + x^3 = f\cos(t).$$

Notice that α in the Duffing equation is negative, which can be considered to be a system of one particle moving in a double-well potential energy. We try 0.3, 0.35, 0.357 and 0.4 for the ratio of driving force to mass, f.

Worksheet 4.9 After solving the differential equation numerically, we use the `odeplot` command to produce x–t plot, the time series, and x–$\dot{x}$ plot, the phase trajectory. This worksheet introduces another representation of a dynamic system – the Poincaré section. Rather than plotting a trajectory in the x–$\dot{x}$ space continuously, the Poincaré section corresponds

to sampling the state of the system at an interval of the period of the driving force. In this example, we discard the first 25 periods to eliminate the transient effect.

```
> Eq1 := diff(x(t),t$2) + b/m*diff(x(t),t) + alpha*x(t)
> + beta*x(t)^3 = F0/m*cos(omega*t);
```

$$Eq1 := \left(\frac{d^2}{dt^2}\,\mathrm{x}(t)\right) + \frac{b\left(\frac{d}{dt}\,\mathrm{x}(t)\right)}{m} + \alpha\,\mathrm{x}(t) + \beta\,\mathrm{x}(t)^3 = \frac{F0\cos(\omega\,t)}{m}$$

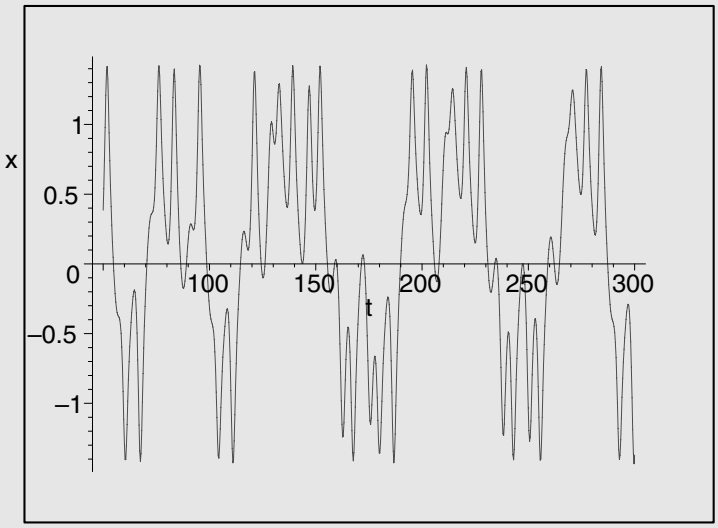
```
> m := 1; b := 0.5; alpha := -1; beta := 1; omega := 1; F0 := 0.4;
```

$$m := 1$$
$$b := 0.5$$
$$\alpha := -1$$
$$\beta := 1$$
$$\omega := 1$$
$$F0 := 0.4$$

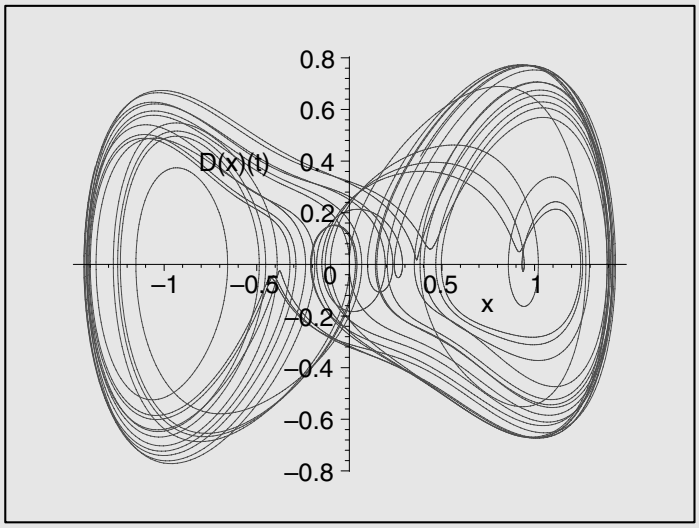
```
> Soln1 := dsolve({Eq1, x(0)=0.4, D(x)(0)=0}, x(t), type=numeric,
> output=listprocedure, maxfun=-1);
```

$$Soln1 := [t = (\mathbf{proc}(t) \ldots \mathbf{end\ proc}),\ \mathrm{x}(t) = (\mathbf{proc}(t) \ldots \mathbf{end\ proc}),$$
$$\frac{d}{dt}\,\mathrm{x}(t) = (\mathbf{proc}(t) \ldots \mathbf{end\ proc})]$$

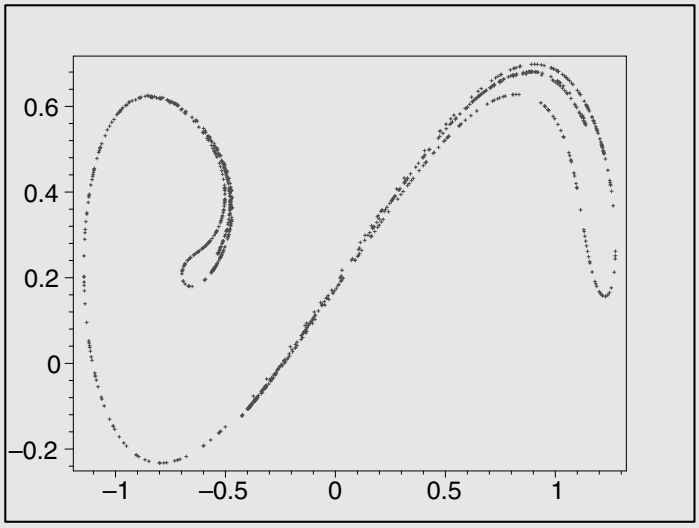
```
> with(plots):
Warning, the name changecoords has been redefined
> odeplot(Soln1, [t, x(t)], 50..300, numpoints=800);
```



```
> odeplot(Soln1, [x(t), D(x)(t)], t=50..300, numpoints=8000);
```




```
> plot([seq([rhs(Soln1(2*Pi*i/omega)[2]),
> rhs(Soln1(2*Pi*i/omega)[3])], i=26..1000)], style=point,
axes=boxed);
```



From Figure 4.5, we see that when f is small, the particle oscillates with a single period equal to the driving period. When $f = 0.35$, it takes two driving periods to complete a full cycle. After gradually increasing f, we discover an oscillating period of four driving periods, and so on. This period-doubling behavior is refereed to as *bifurcation*. At $f = 0.4$, the trajectory

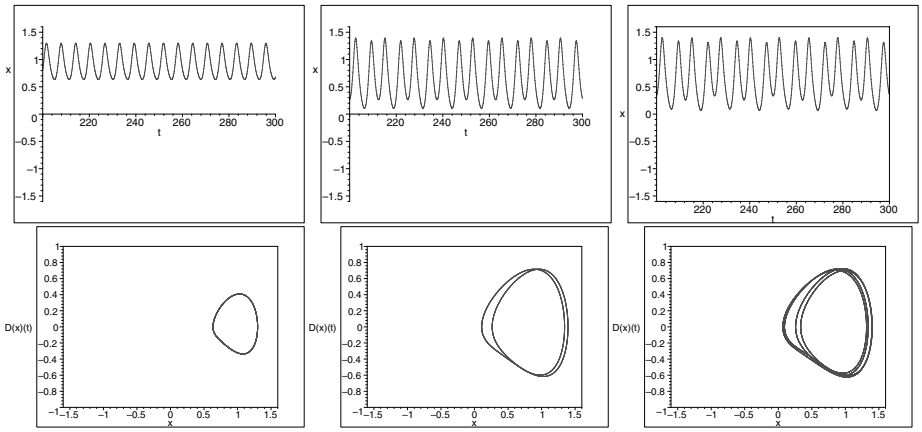


Figure 4.5: The time series and trajectories of the Duffing equation with different values for the driving force f. A period-1 orbit occurs when $f = 0.3$ (a); a period-2 orbit occurs when $f = 0.35$ (b); a period-4 orbit occurs when $f = 0.357$ (c).

appears to be chaotic. In addition to the time series and phase trajectory, the Poincaré section serves as another useful technique which can be used to examine a nonlinear system. The Poincaré section is a collection of x and $\dot{x}$ of a system sampled at certain intervals. In the example of the Duffing equation, each time when $\omega t = 2\pi$, it marks a point in the x–$\dot{x}$ plane. The reader can verify that for a period-1 motion, the Poincaré section is simply a point, and for a period-n motion, it gives n points. For a seemingly chaotic motion, a pattern might gradually emerge in a Poincaré section. What we saw in the worksheet is called a *strange attractor*, and we will leave it to other textbooks or articles to explain the details of the chaotic systems.[3] One should systematically scan through different values of f to observe properties of a nonlinear oscillator. The "period-doubling route to chaos" which we observed, is common in many nonlinear systems.

4.6 Summary of Lagrangian Mechanics

We devote much of this chapter to the Lagrangian formulation of mechanics; a great advantage of this approach is that we treat the energy, which is a scalar quantity, instead of the force, which is a vector, with typically three components for each particle. Once the Lagrangian is obtained, the derivation of equations of motion is straightforward. In implementing Lagrangian mechanics, Maple simplifies expressions of kinetic energy and potential energy in terms of generalized coordinates, and performs required differentiations, which are generally tedious even for a simple system with only two degrees of freedom. Furthermore,

[3] See, e.g., Marion and Thornton 1995, Chapter 4.

Maple makes necessary rearrangements of equations of motion, which are typically a system of coupled differential equations. Solving differential equations numerically, Maple readily produces graphical results of solutions; by experimenting with various configurations and initial conditions, one acquires a profound intuition about the underlying physics. With basic Maple commands `subs`, `diff` and `dsolve`, essentially any problem in classical mechanics are solvable according to the method explained in these two chapters. The reader is encouraged to apply this method in exploring many problems in Chapter 2 of Goldstein et al. 2002.

A Hamiltonian formulation is an alternative representation of classical mechanics in an integral form. Whereas a Lagrangian is expressed as a function of generalized coordinates and their derivatives with respect to time, a Hamiltonian is expressed as a function of generalized coordinates and their conjugate momenta. For solution of mechanical problems, methods involving a Hamiltonian are not superior to those with a Lagrangian; we refrain from further discussion here, but encourage the reader to consult Goldstein (see above) and to apply Maple to the solution of problems using the Hamiltonian techniques. The utility of the Hamiltonian approach is evident in the treatment of quantum mechanics. As we will describe in Chapter 14, an applicable procedure involves forming a classical Hamiltonian, converting to the Schrödinger equation by replacing classical variables with operators, and solving the equation, typically only approximately.

Exercises

1. In the model of a double pendulum in Section 4.2, make numerical experiments according to the following conditions: assume the oscillation to be small; $l_1 = l_2$; m_1 is much greater than m_2 ($m_2 \ll m_1$). Initial conditions are $\theta_1(0) = \theta_2(0) = \dot{\theta}_2(0) = 0$ and $\dot{\theta}_1(0) = v$, which implies m_1 to have been suddenly struck.

2. For a double pendulum with $m_1 = m_2$ and $l_1 = l_2$, use the small-angle approximation to linearize equations (4.8) and (4.9), so that one can find analytic solutions for θ_1 and θ_2. From these solutions one should discover that the pendulum oscillates at a combination of two normal frequencies:

$$\omega_1 = \sqrt{\frac{\left(2+\sqrt{2}\right) g}{l_1}}, \quad \omega_2 = \sqrt{\frac{\left(2-\sqrt{2}\right) g}{l_1}}.$$

   Hint: Let $\cos(\theta_1 - \theta_2) \cong 1$, $\dot{\theta_1}^2 = \dot{\theta_2}^2 \cong 0$, $\sin\theta_1 \cong \theta_1$, and $\sin\theta_2 \cong \theta_2$.

3. Develop a Maple worksheet for a triple pendulum.

4. An inverted pendulum consisting of a bob of mass m and a massless stick of length l is attached to an oscillating table; the position of the table is described by $A\cos\omega t$, where the frequency ω is adjustable; see Figure 4.6.

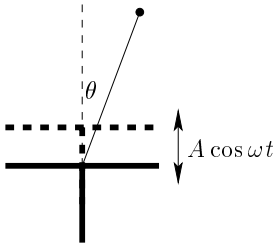


Figure 4.6: An inverted pendulum.

(a) Derive the equation of motion for θ.
Answer: $l\ddot{\theta} + (A\omega^2 \cos\omega t - g)\sin\theta = 0$.

(b) Numerically solve the differential equation using, for example, $l = 0.1$ m, $A = 0.01$ m, $\omega = 90$ s^{-1} or $\omega = 150$ s^{-1}; produce an animation similar to the worksheet in Section 4.2. Observe that when ω is large enough, the pendulum will not fall over.

5. Derive from equation (4.29) to equation (4.30a) using

$$\tan^{-1} x = \frac{\pi}{2} - \cos^{-1} \frac{x}{\sqrt{x^2+1}}. \tag{4.57}$$

6. Prove that, if a particle moves under the influence of potential energy

$$V(r) = -\frac{k}{r} + \frac{h}{r^2}, \tag{4.58}$$

the trajectory of the particle can be described as

$$r = \frac{s^2}{mk} \frac{1}{1 + \epsilon\cos\left(\frac{s}{l}\phi\right)}, \tag{4.59}$$

where

$$s \equiv \sqrt{l^2 + 2mh}, \quad \epsilon \equiv \sqrt{1 + \frac{2Es^2}{mk^2}}. \tag{4.60}$$

7. (a) In the preceding exercise, if $h = 0$, we have a function (neglecting a factor l^2/mk)

$$r = \frac{1}{1 + \epsilon\cos\phi},$$

which is the solution of the Kepler problem. Use the `polarplot` command to plot this function for $\epsilon = 0, 0.44, 1, 1.25$. Do the results correspond to a circle, an ellipse, a parabola and a hyperbola respectively?

(b) Suppose h to be small, so that $s \cong l$, but $s/l = 1.02$; plot

$$r = \frac{1}{1 + 0.44\cos(1.02\phi)}.$$

One expects this plot to demonstrate precession when a small term proportional to r^{-2} is added to a pure r^{-1} potential.

8. The orbit shown on the front cover of Goldstein's *Classical Mechanics* (second edition and early third edition) is impossible![4] For bounded motion under an attractive central force, the orbit at a turning point must always be concave towards the center of force (Goldstein had it concave outwards). Consider the potential for Figure 3–13 on p. 91 of Goldstein's book,

$$V = \frac{r^{23}}{23}; \tag{4.61}$$

let, for example,

$$r_0 = 1, \quad \dot{r}_0 = 0.1, \quad \phi_0 = 0, \quad \dot{\phi}_0 = 1,$$

so that the energy and the angular momentum are

$$E = 0.548, \quad l = 1.$$

Use Maple to produce the correct plot of the orbit, which should resemble Figure 4.7.

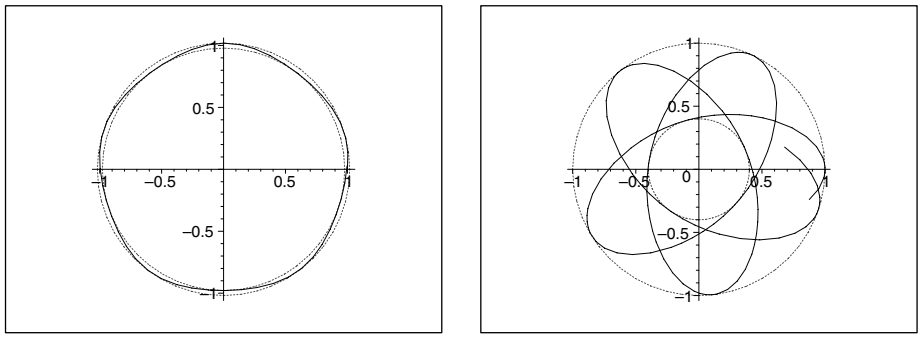


Figure 4.7: Orbits for bounded motion under attractive central forces (a) $V \propto r^{23}$; (b) $V \propto r^{7/9}$.

[4]M. Tiersten, "Errors in Goldstein's *Classical Mechanics*," *American Journal of Physics*, **71**, 103 (2003).

9. For an asymmetric top with $I_1 = 65.3$ kg m^2, $I_2 = 50.3$ kg m^2, and $I_3 = 25.1$ kg m^2, consider its motion in the absence of gravity. For example, try the initial values $\phi_0 = 0$, $\dot{\phi}_0 = 0.5$ rad s^{-1}, $\theta_0 = \pi/2$, $\dot{\theta}_0 = 0.25$ rad s^{-1}, $\psi_0 = 0$, and $\dot{\psi}_0 = 1.0$ rad s^{-1}. From Figure 4.8, one can see that the angular velocity vector $\boldsymbol{\omega}$ returns to its original position, but the top itself does not return to its original position.

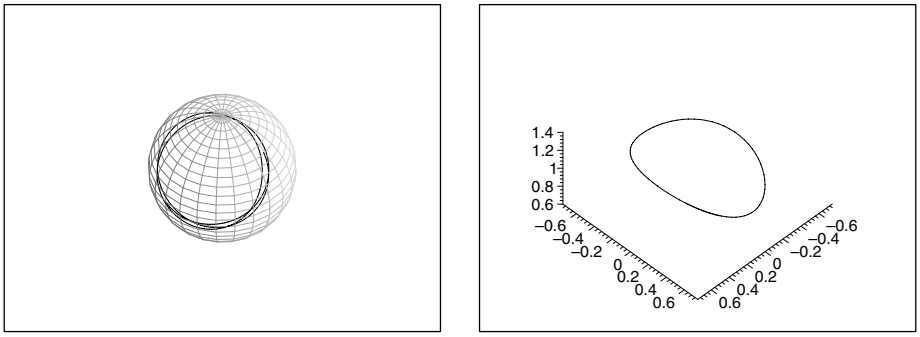


Figure 4.8: Motion of an asymmetric top in the absence of gravity. (a) Trajectory of a point on the body z axis relative to the fixed system of coordinates; (b) trajectory of the angular velocity vector $\boldsymbol{\omega}$.

10. For the Duffing equation

$$\ddot{x} + \gamma\dot{x} + \alpha x + \beta x^3 = f\cos(\omega t)$$

with $\gamma = 0.2$, $\alpha = 1$, $\beta = 1$ and $F = 25$, scan the frequency range from $\omega = 1.26$ to $\omega = 1.29$ to find the period-doubling transitions (bifurcations).

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5 Orthogonal Functions and Expansions

Representation of a function as an expansion in orthogonal functions is an important topic in mathematical physics. We require this technique in studying the theory of potential, waves and quantum mechanics in subsequent chapters. In this chapter we begin with the familiar Fourier series and Fourier integrals; we then extend our treatment to two other orthogonal functions: the Legendre functions and Bessel functions. Maple defines these special functions that one can readily invoke to find their roots, to evaluate expansion coefficients and to produce graphs.

5.1 Fourier Series

The best known orthogonal functions are sines and cosines; an expansion in their terms constitutes a Fourier series. Such a series can apply to a periodic function, or to a function defined on an interval.

A function $u(x)$ is periodic with period $L > 0$ if

$$u(x + L) = u(x). \tag{5.1}$$

Without a rigorous proof, we state that any continuous function $u(x)$ that is periodic with period L, or a function that is defined on an interval $[0, L]$, can be expressed as

$$u(x) = \sum_{m=0}^{\infty} \left[a_m \cos(mkx) + b_m \sin(mkx) \right], \tag{5.2}$$

or explicitly

$$\begin{aligned} u(x) = \quad & a_0 \\ & + a_1 \cos(kx) \quad + b_1 \sin(kx) \\ & + a_2 \cos(2kx) \quad + b_2 \sin(2kx) \\ & + a_3 \cos(3kx) \quad + b_3 \sin(3kx) \\ & + \ldots \qquad\quad + \ldots, \end{aligned} \tag{5.2′}$$

where

$$k = \frac{2\pi}{L}. \tag{5.3}$$

Physics with Maple™: The Computer Algebra Resource for Mathematical Methods in Physics. Frank Y. Wang
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ISBN: 3-527-40640-9

Although there exist functions that admit no expansion as a Fourier series, for most functions of interest in physics we assume the existence of such an expansion.

Fourier coefficients are evaluated through these integrals:

$$a_0 = \frac{1}{L}\int_0^L u(x)\,dx, \tag{5.4}$$

$$a_n = \frac{2}{L}\int_0^L u(x)\cos(nkx)\,dx, \tag{5.5}$$

$$b_n = \frac{2}{L}\int_0^L u(x)\sin(nkx)\,dx. \tag{5.6}$$

We must be aware that the integral for a_0 differs from that for other a_n by a factor of 2. In some literature, the series begins with $a_0/2$, so that the integral for a_0 has the same form as that for other a_n. Take care with the definition.

Example 5.1 Expand the square wave as a Fourier series. A square wave is described as

$$u(x) = \begin{cases} 1, & 0 < x < \dfrac{L}{2}; \\ -1, & \dfrac{L}{2} < x < L. \end{cases} \tag{5.7}$$

Suppose that $u(x + L) = u(x)$.

Solution One can perform a direct calculation to verify that a_m are zero; the reason is that the given function is odd, and $\cos(mkx)$ are even. The coefficients b_m are evaluated by

$$b_m = \frac{1}{L}\left[\int_0^{L/2} \sin(mkx)\,dx - \int_{L/2}^{L} \sin(mkx)\,dx\right] = 2\frac{1-(-1)^m}{m\pi}.$$

Only when m is odd do the b_m not vanish. This function hence is written as

$$u(x) = \frac{4}{\pi}\sum_{m=1,3,5,\ldots} \frac{1}{m}\sin\frac{2m\pi x}{L}. \tag{5.8}$$

Worksheet 5.1 Evaluation of the Fourier coefficients for a square wave is easy. We use the `assuming` option after the `int` command in Maple to ensure that n is treated as an integer.

```
> k := 2*Pi/L;
```

$$k := \frac{2\,\pi}{L}$$

```
> bm := 2/L*(int(sin(m*k*x), x=0..L/2) + int(-sin(m*k*x),
> x=L/2..L)) assuming m::integer;
```

$$bm := -\frac{2\,((-1)^m - 1)}{m\,\pi}$$

Example 5.2 Find the Fourier series for a function

$$u(x) = \begin{cases} x, & 0 < x < 1, \\ \dfrac{3}{2} - \dfrac{x}{2}, & 1 < x < 3. \end{cases} \tag{5.9}$$

Suppose that $u(x+3) = u(x)$.

Solution According to the definition, we directly write

$$L = 3, \quad k = \frac{2\pi}{3}.$$

The Fourier coefficients are hence

$$a_0 = \frac{1}{3}\int_0^1 x dx + \frac{1}{3}\int_1^3 \left(\frac{3}{2} + \frac{x}{2}\right) dx,$$

$$a_m = \frac{2}{3}\int_0^1 x\cos(mkx)\, dx + \frac{2}{3}\int_1^3 \left(\frac{3}{2} + \frac{x}{2}\right)\cos(mkx)\, dx,$$

$$b_m = \frac{2}{3}\int_0^1 x\sin(mkx)\, dx + \frac{2}{3}\int_1^3 \left(\frac{3}{2} + \frac{x}{2}\right)\sin(mkx)\, dx.$$

Maple performs these integrations; the function $u(x)$ is represented as

$$u(x) = \sum_{m=0}^{N} [a_m \cos(mkx) + b_m \sin(mkx)]. \tag{5.10}$$

For practical applications we truncate the series at the Nth term, according to our desired precision. To write the series explicitly, we have

$$u(x) = \frac{1}{2} - \frac{27}{8\pi^2}\cos\frac{2\pi x}{3} + \frac{9\sqrt{3}}{8\pi^2}\sin\frac{2\pi x}{3} - \frac{27}{32\pi^2}\cos\frac{4\pi x}{3} + \frac{9\sqrt{3}}{32\pi^2}\sin\frac{4\pi x}{3} + \ldots.$$

Worksheet 5.2 When we undertake integration repeatedly, a `for` loop, which is a basic programming construct, is convenient.

```
> L := 3:
> k := 2*Pi/L;
```

$$k := \frac{2\,\pi}{3}$$

```
> a[0] := 1/L*(int(x, x=0..1) + int((3/2-x/2), x=1..3));
```

$$a_0 := \frac{1}{2}$$

```
> N := 5:
```

```
> for m from 1 to N do
> a[m] := 2/L*simplify(int(x*cos(m*k*x), x=0..1) +
> int((3/2-x/2)*cos(m*k*x), x=1..3));
> end do;
```

$$a_1 := -\frac{27}{8\,\pi^2}$$

$$a_2 := -\frac{27}{32\,\pi^2}$$

$$a_3 := 0$$

$$a_4 := -\frac{27}{128\,\pi^2}$$

$$a_5 := -\frac{27}{200\,\pi^2}$$

```
> for m from 1 to N do
> b[m] := 2/L*simplify(int(x*sin(m*k*x), x=0..1) +
> int((3/2-x/2)*sin(m*k*x), x=1..3));
> end do;
```

$$b_1 := \frac{9\sqrt{3}}{8\,\pi^2}$$

$$b_2 := -\frac{9\sqrt{3}}{32\,\pi^2}$$

$$b_3 := 0$$

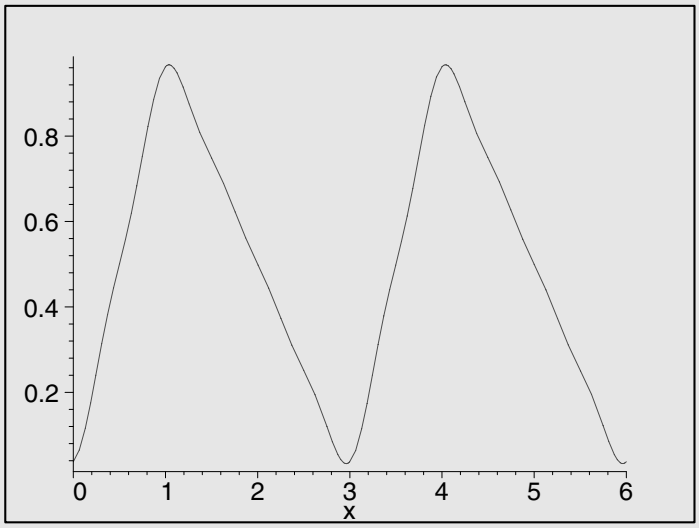
$$b_4 := \frac{9\sqrt{3}}{128\,\pi^2}$$

$$b_5 := -\frac{9\sqrt{3}}{200\,\pi^2}$$

```
> Epr1 := a[0] + add(a[m]*cos(m*k*x), m=1..N) +
add(b[m]*sin(m*k*x),
> m=1..N);
```

$$\begin{aligned} Epr1 := {} & \frac{1}{2} - \frac{27}{8}\,\frac{\cos\left(\frac{2\,\pi\,x}{3}\right)}{\pi^2} - \frac{27}{32}\,\frac{\cos\left(\frac{4\,\pi\,x}{3}\right)}{\pi^2} - \frac{27}{128}\,\frac{\cos\left(\frac{8\,\pi\,x}{3}\right)}{\pi^2} \\ & - \frac{27}{200}\,\frac{\cos\left(\frac{10\,\pi\,x}{3}\right)}{\pi^2} + \frac{9}{8}\,\frac{\sqrt{3}\sin\left(\frac{2\,\pi\,x}{3}\right)}{\pi^2} - \frac{9}{32}\,\frac{\sqrt{3}\sin\left(\frac{4\,\pi\,x}{3}\right)}{\pi^2} \\ & + \frac{9}{128}\,\frac{\sqrt{3}\sin\left(\frac{8\,\pi\,x}{3}\right)}{\pi^2} - \frac{9}{200}\,\frac{\sqrt{3}\sin\left(\frac{10\,\pi\,x}{3}\right)}{\pi^2} \end{aligned}$$

```
> plot(Epr1, x=0..2*L);
```



The most intuitive way to test the correctness of an expansion is to observe the series graphically. In this example, the original function has a sawtooth shape; according to the plot the Fourier series satisfactorily represents this function.

5.2 Fourier Integrals

The Fourier series applies to a periodic function or to a function defined on an interval $[0, L]$. It is possible to generalize the expansion for a non-periodic function over any specified finite range. To do so we replace the summation in the Fourier series by an integral, so that a function $u(x)$ becomes a Fourier integral,

$$u(x) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \alpha(k) e^{ikx} dk, \tag{5.11}$$

where

$$\alpha(k) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} u(x) e^{-ikx}\, dx. \tag{5.12}$$

The function $\alpha(k)$ is called the Fourier transform of $u(x)$, and it corresponds to Fourier coefficients in the Fourier series. Notice that this definition of Fourier transform differs from that in Maple's `inttrans` package; in this chapter we do not invoke that Maple package, but perform the integration directly.

Example 5.3 Find the Fourier transform $\alpha(k)$ for a function

$$u(x) = \begin{cases} 1, & -\frac{1}{2} < x < \frac{1}{2}, \\ 0, & x < -\frac{1}{2},\ x > \frac{1}{2}. \end{cases} \tag{5.13}$$

Solution The integral is straightforward:

$$\alpha(k) = \frac{1}{(2\pi)^{1/2}} \int_{-1/2}^{1/2} e^{-ikx}\, dx = \sqrt{\frac{2}{\pi}} \frac{\sin\frac{k}{2}}{k}. \tag{5.14}$$

We write $u(x)$ as a Fourier integral. For practical use, we choose the truncation limit at k_0, and write the integral as

$$u(x) = \frac{1}{(2\pi)^{1/2}} \int_{-k_0}^{k_0} \sqrt{\frac{2}{\pi}} \frac{\sin\frac{k}{2}}{k} e^{ikx} dk, \tag{5.15}$$

where k_0 depends on our desired precision.

Worksheet 5.3 We employ the `piecewise` command to produce the function $u(x)$ for graphic purposes. This worksheet directly follows the definition of the Fourier integral. As the Fourier integral involves integration with complex numbers, we employ the `evalc` command to simplify the expression.

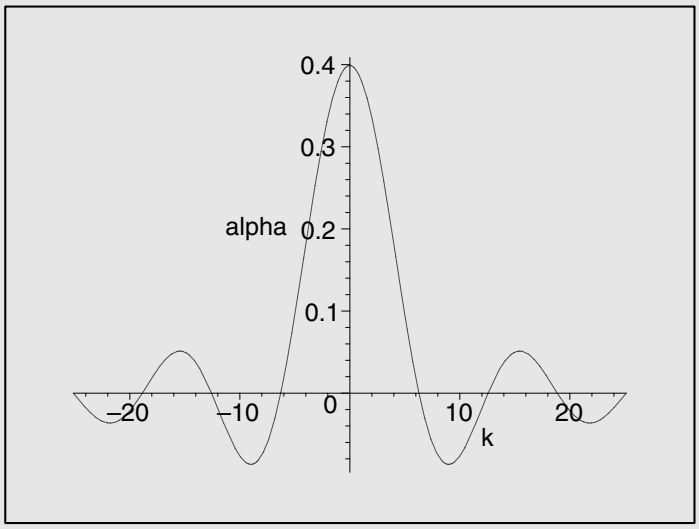
```
> u := piecewise(-1/2<x and x<1/2, 1, x<-1/2, 0, 1/2<x, 0):
> alpha := 1/sqrt(2*Pi)*int(1*exp(-I*k*x), x=-1/2..1/2);
```

$$\alpha := \frac{\frac{1}{2} I \sqrt{2} \left(e^{(-1/2\, I\, k)} - e^{(1/2\, I\, k)}\right)}{\sqrt{\pi}\, k}$$

```
> alpha := simplify(alpha);
```

$$\alpha := \frac{\sqrt{2} \sin(\frac{1}{2} k)}{\sqrt{\pi}\, k}$$

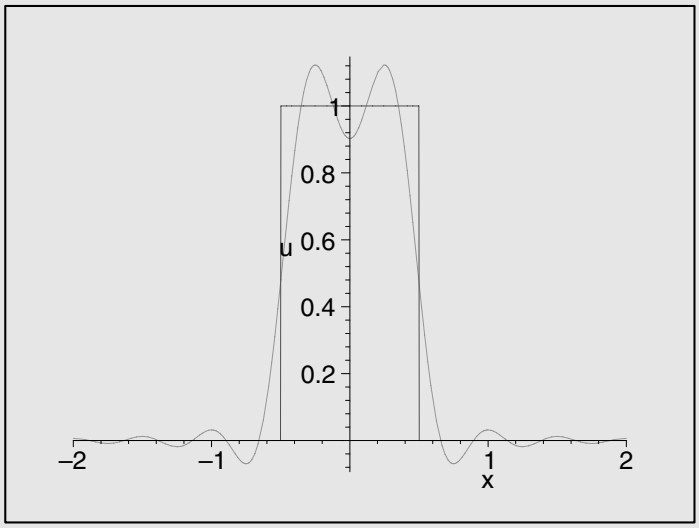
```
> plot(alpha, k=-8*Pi..8*Pi, labels=["k", "alpha"]);
```




```
> Epr1 := 1/sqrt(2*Pi)*int(alpha*exp(I*k*x), k=-4*Pi..4*Pi);
```

$$Epr1 := \frac{1}{2}\,\frac{\sqrt{2}\displaystyle\int_{-4\,\pi}^{4\,\pi}\frac{\sqrt{2}\sin(\frac{1}{2}\,k)\,e^{(I\,k\,x)}}{\sqrt{\pi}\,k}\,dk}{\sqrt{\pi}}$$

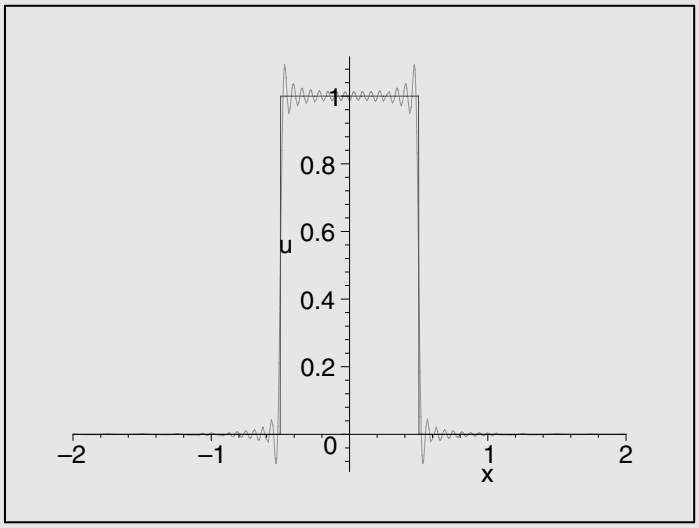
```
> Epr2 := simplify(Epr1):
> Epr3 := evalc(Epr2):
> Epr4 := simplify(Epr3):
> plot({u, Epr4}, x=-2..2, labels=["x", "u"]);
```



```
> Epr5 := 1/sqrt(2*Pi)*int(alpha*exp(I*k*x), k=-32*Pi..32*Pi);
```

$$Epr5 := \frac{1}{2}\,\frac{\sqrt{2}\displaystyle\int_{-32\,\pi}^{32\,\pi}\frac{\sqrt{2}\sin(\frac{1}{2}\,k)\,e^{(I\,k\,x)}}{\sqrt{\pi}\,k}\,dk}{\sqrt{\pi}}$$

```
> Epr6 := simplify(Epr5):
> Epr7 := evalc(Epr6):
> Epr8 := simplify(Epr7):
> plot({u, Epr8}, x=-2..2, labels=["x", "u"]);
```



The exact Fourier integral is typically difficult to evaluate. We demonstrate two limits that we choose for k_0; obviously a larger k_0 gives a more accurate representation of $f(x)$. Near the points of discontinuity, we recognize rapid oscillation; this behavior is known as the Gibbs phenomenon.

5.3 Orthogonal Functions in Complete Sets

Consider a set of real or complex functions $f_n(x)$, $n = 1, 2, \ldots$, square integrable on an interval $[a, b]$ for a variable x; this set is defined to be orthonormal if

$$\int_a^b f_n^*(x) f_m(x) dx = \delta_{nm}, \tag{5.16}$$

where δ_{nm} is the Kronecker delta. The completeness (or closure) relation is

$$\sum_{n=1}^{\infty} f_n^*(x')f_n(x) = \delta(x' - x), \tag{5.17}$$

where $\delta(x' - x)$ is the Dirac delta function. The asterisk denotes the complex conjugate, although in this chapter we are concerned with real functions only. If we have an arbitrary function $u(x)$, square integrable on the interval $[a, b]$, we can expand it in a series of orthonormal functions $f_n(x)$,

$$u(x) = \sum_{n=1}^{\infty} c_n f_n(x), \tag{5.18}$$

where expansion coefficients are evaluated as

$$c_n = \int_a^b f_n^*(x)u(x)dx. \tag{5.19}$$

In the Fourier series discussed in Section 5.1, these sets of orthogonal functions are sines and cosines, on the interval $[0, L]$. We proceed to introduce other orthogonal functions.

5.4 Legendre Polynomials

The Legendre equation is

$$(1 - x^2)\frac{d^2P}{dx^2} - 2x\frac{dP}{dx} + l(l + 1)P = 0. \tag{5.20}$$

To solve this equation, we can write P as a power series, then we determine the coefficients that satisfy the differential equations; such a technique is discussed in Appendix B.1. If our only concern is applications, the solutions of this equation are well established. When l is 0 or a positive integer, the solutions are called the Legendre polynomials, which are defined as `LegendreP` in Maple.

Worksheet 5.4 We invoke the `LegendreP` command, and use the `expand` command to display the Legendre polynomials explicitly. Their plots are shown in the worksheet.

```
> p[0] := expand(LegendreP(0,x)); p[1] := expand(LegendreP(1, x));
> p[2] := expand(LegendreP(2, x)); p[3] := expand(LegendreP(3, x));
> p[4] := expand(LegendreP(4, x)); p[5] := expand(LegendreP(5, x));
```

$$p_0 := 1$$
$$p_1 := x$$

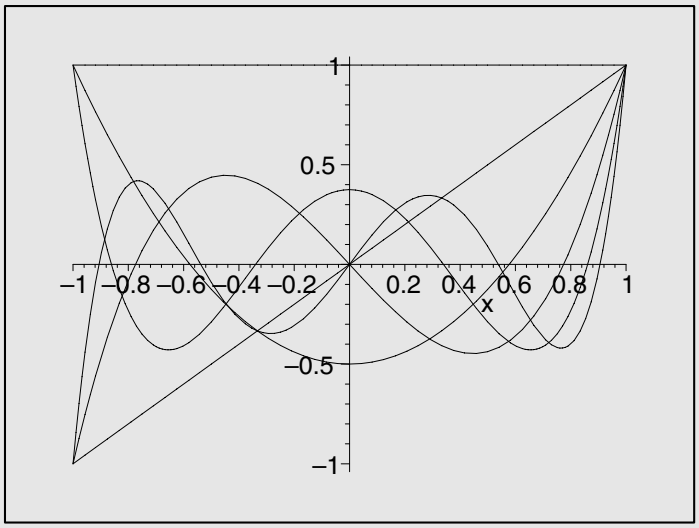
$$p_2 := -\frac{1}{2} + \frac{3\,x^2}{2}$$

$$p_3 := \frac{5}{2}\,x^3 - \frac{3}{2}\,x$$

$$p_4 := \frac{3}{8} + \frac{35}{8}\,x^4 - \frac{15}{4}\,x^2$$

$$p_5 := \frac{63}{8}\,x^5 - \frac{35}{4}\,x^3 + \frac{15}{8}\,x$$

```
> plot({seq(p[i], i=0..5)}, x=-1..1);
```



The first few Legendre polynomials are listed in Table 5.1. We see that P_l is a polynomial of degree l; it is an even function if l is even, and is an odd function if l is odd.

Legendre polynomials form a complete set of orthogonal functions on the interval $(-1, 1)$. The condition for Legendre polynomials to be orthogonal is

$$\int_{-1}^{1} P_{l'}(x) P_l(x) dx = \frac{2}{2l+1} \delta_{l'l}. \tag{5.21}$$

The difference between orthogonal functions and orthonormal functions is just an overall scaling factor. If we rescale P_l as

$$f_l = \sqrt{\frac{2l+1}{2}} P_l,$$

we obtain a set of orthonormal functions f_l. Be aware that the definition of orthogonal functions might differ by a constant factor in different literature. If we expand a function in un-

Table 5.1: Legendre polynomials.

l	$P_l(x)$
0	1
1	x
2	$\frac{3}{2}x^2 - \frac{1}{2}$
3	$\frac{5}{2}x^3 - \frac{3}{2}x$
4	$\frac{35}{8}x^4 - \frac{15}{4}x^2 + \frac{3}{8}$
5	$\frac{63}{8}x^5 - \frac{35}{4}x^3 + \frac{15}{8}x$

normalized orthogonal functions, we only need to adjust the expansion coefficients to impose normalization.

A function on an interval $(-1, 1)$ can be expanded as Legendre polynomials,

$$u(x) = \sum_{l=0}^{\infty} A_l P_l(x), \tag{5.22}$$

or explicitly,

$$u(x) = A_0 + A_1 x + A_2 \left(\frac{3}{2}x^2 - \frac{1}{2}\right) + A_3 \left(\frac{5}{2}x^3 - \frac{3}{2}x\right) + \dots. \tag{5.22$'$}$$

The coefficients are evaluated according to this integral,

$$A_l = \frac{2l+1}{2} \int_{-1}^{1} u(x) P_l(x) dx. \tag{5.23}$$

Notice the scaling factor before the integral, which arises from our use of unnormalized orthogonal functions.

Example 5.4 Expand this function,

$$u(x) = \begin{cases} -1, & -1 < x < 0, \\ 1, & 0 < x < 1, \end{cases} \tag{5.24}$$

in Legendre polynomials.

Solution To calculate the coefficients, we perform the integration:

$$A_l = \frac{2l+1}{2} \left(\int_{-1}^{0} P_l \, dx - \int_{0}^{1} P_l \, dx \right).$$

Maple directly accomplishes this simple task. The fact that even terms vanish is explained by symmetry: we are expanding an odd function.

We can express $u(x)$ as

$$u(x) = \frac{3}{2}x - \frac{7}{8}\left(\frac{5}{2}x^3 - \frac{3}{2}x\right) + \frac{11}{16}\left(\frac{63}{8}x^5 - \frac{35}{4}x^3 + \frac{15}{8}x\right) + \ldots .$$

Worksheet 5.5 The procedure for evaluating expansion coefficients here is identical to that for the Fourier series: we merely replace `sin` or `cos` with `LegendreP`. We again employ a `for` loop to perform repeated evaluation of integrals.

```
> N := 19:
> for l from 0 to N do
> A[l] := (2*l + 1)/2*simplify(int(LegendreP(l,x), x=0..1) -
> int(LegendreP(l,x),x=-1..0));
> end do;
```

$$A_0 := 0$$
$$A_1 := \frac{3}{2}$$
$$A_2 := 0$$
$$A_3 := \frac{-7}{8}$$
$$A_4 := 0$$
$$A_5 := \frac{11}{16}$$
$$A_6 := 0$$
$$A_7 := \frac{-75}{128}$$
$$A_8 := 0$$
$$A_9 := \frac{133}{256}$$
$$A_{10} := 0$$
$$A_{11} := \frac{-483}{1024}$$
$$A_{12} := 0$$
$$A_{13} := \frac{891}{2048}$$
$$A_{14} := 0$$
$$A_{15} := \frac{-13299}{32768}$$

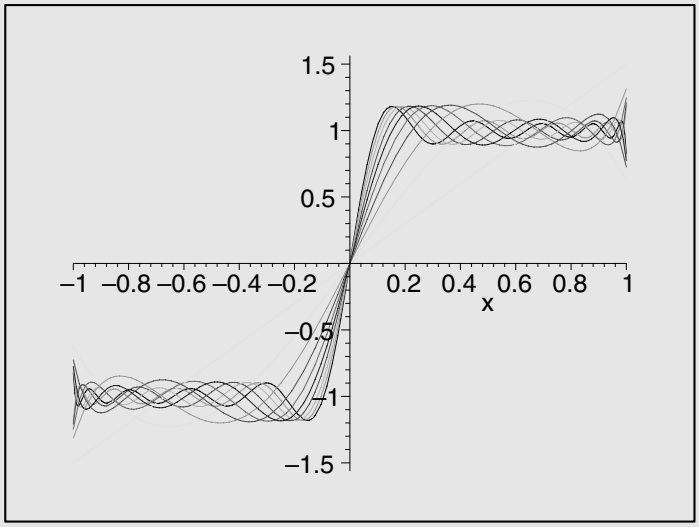
$$A_{16} := 0$$

$$A_{17} := \frac{25025}{65536}$$

$$A_{18} := 0$$

$$A_{19} := \frac{-94809}{262144}$$

```
> f := n -> add(A[l]*LegendreP(l,x), l=0..n):
> with(plots):
Warning, the name changecoords has been redefined
> p1 := plot({seq(f(n), n=1..N-1)}, x=-1..1):
> p2 := plot(f(N), x=-1..1, thickness=2, color=black):
> display([p1, p2]);
```



We plot the progressive improvement in the representation of a square wave in Legendre polynomials. Not surprisingly, the more terms that we include, the more accurate is the result.

5.4.1 Generating Function and Rodrigues Formula

There are multiple ways to define the Legendre polynomials (and most orthogonal polynomials). Although the Legendre polynomials are known as solutions of the Legendre equation, one can alternatively define the Legendre polynomials by the generating function:

$$\psi(x,t) = \frac{1}{\sqrt{1-2xt+t^2}}. \tag{5.25}$$

Expanding this function as a power series of t, one obtains

$$\frac{1}{\sqrt{1-2xt+t^2}} = \sum_{l=0}^{\infty} P_l(x)t^l, \quad (0 < t < 1). \tag{5.26}$$

Generating functions are available for most orthogonal polynomials (see two exercises at the end of the chapter), but that for the Legendre polynomials has a simple geometrical meaning, which will be evident in Section 6.4.2.

Worksheet 5.6 We use the `taylor` command to expand the generating function for the Legendre polynomials.

```
> gen := 1/sqrt(1 - 2*x*t + t^2);
```

$$gen := \frac{1}{\sqrt{1-2\,x\,t+t^2}}$$

```
> taylor(gen, t);
```

$$1 + x\,t + \left(-\frac{1}{2} + \frac{3\,x^2}{2}\right) t^2 + \left(-\frac{3}{2}\,x + \frac{5}{2}\,x^3\right) t^3 + \left(\frac{3}{8} - \frac{15}{4}\,x^2 + \frac{35}{8}\,x^4\right) t^4 + \left(\frac{15}{8}\,x - \frac{35}{4}\,x^3 + \frac{63}{8}\,x^5\right) t^5 + \mathrm{O}\left(t^6\right)$$

From the Maple output, we see that the coefficients of t^l are indeed the Legendre polynomials $P_l(x)$. The generating function gives an implicit formula for the Legendre polynomials. There is yet another way to define the Legendre polynomials:

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l. \tag{5.27}$$

This is Rodrigues' explicit formula for the Legendre polynomials. We leave it as an exercise for the reader to use Maple to perform this simple differentiation; one can also find an example in Section 16.2. For some orthogonal polynomials, conventions of a constant factor vary in the literature; the generating function which Rodrigues' provides allows us to check the definition between different sources.

5.5 Bessel Functions

The differential equation

$$\rho^2\frac{d^2J}{d\rho^2} + \rho\frac{dJ}{d\rho} + (\rho^2 - \nu^2)J = 0 \tag{5.28}$$

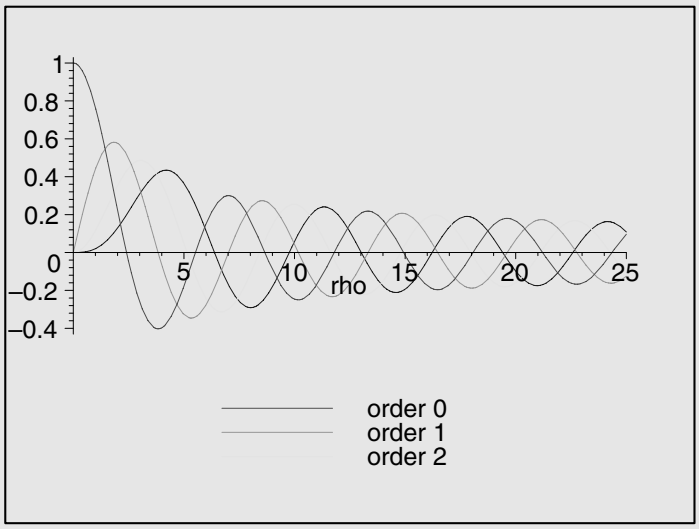
is called the Bessel equation of order ν. Solutions of this equation are also well established, called Bessel functions of order ν. There are exhaustive treatments of this subject; as the solution lacks a simple algebraic expression, one traditionally needs to consult reference books to retrieve numerical properties of Bessel functions, such as their roots. Maple reduces routines of numerical methods for Bessel functions to simple commands, which is extremely useful in practical computation.

The Bessel equation is a second-order differential equation, for which there are two linearly independent solutions; they can be linearly combined in various ways. In Section 1.4.2 we have plotted these two functions: `BesselJ` and `BesselY`. For many physical applications, we choose `BesselJ` only, because it is finite at the origin. We commonly refer to it as the Bessel function of the first kind, of order ν, generally denoted $J_\nu(\rho)$ in the literature.

We graphically present $J_\nu(\rho)$ for orders ν from zero to three.

Worksheet 5.7 In Maple, the Bessel functions $J_\nu(\rho)$ are entered as `BesselJ(nu, rho)`.

```
> plot([BesselJ(0, rho), BesselJ(1, rho), BesselJ(2, rho),
> BesselJ(3, rho)], rho=0..25, legend=["order 0", "order 1",
> "order 2", "order 3"]);
```



In almost all problems, we need to find roots of Bessel functions. Graphically, roots correspond to points at which the curve crosses the x axis. These roots can be obtained by a numerical method, which can be accomplished with Maple; indeed Maple has a command `BesselJZeros` specifically for this purpose. We offer examples of how to find the roots in subsequent worksheets; here we list some of them in Table 5.2.

Table 5.2: Roots $x_{\nu n}$ of Bessel functions for which $J_\nu(x_{\nu n}) = 0$.

n	ν		
	0	1	2
1	2.405	3.832	5.136
2	5.520	7.016	8.417
3	8.654	10.173	11.620
4	11.792	13.324	14.796
5	14.931	16.471	17.960

We label these roots with index n as $x_{\nu n}$: for fixed ν (the order of a Bessel function),

$$x_{\nu 1} < x_{\nu 2} < x_{\nu 3} \ldots .$$

Pay attention to the notation of indices, ν and n, which we will discuss below.

For order ν to be a non-negative integer, the Bessel function of that order satisfies the orthogonality condition on an interval $(0, a)$,

$$\int_0^a \rho J_\nu \left(x_{\nu n'} \frac{\rho}{a} \right) J_\nu \left(x_{\nu n} \frac{\rho}{a} \right) d\rho = \frac{a^2}{2} [J_{\nu+1}(x_{\nu n})]^2 \delta_{n'n}. \tag{5.29}$$

In this equation we extend the definition of orthogonality in equation (5.16) to a more general form,

$$\int_0^a w(x) f_n^*(x) f_m(x) dx = \delta_{nm}, \tag{5.30}$$

where we insert a weight function w. In our example of Bessel functions, the weight function is $w = \rho$.

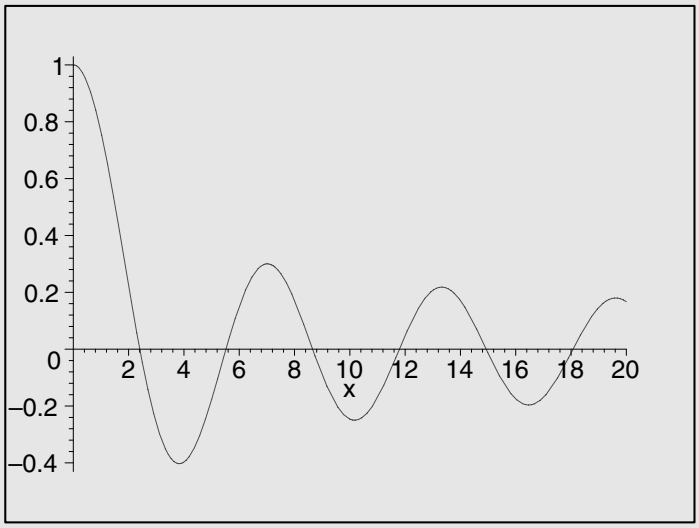
Be aware of indices: ν is the order of the Bessel function, and n is the nth root of the Bessel function. The orthogonal condition applies to a function with fixed ν. For example, if $\nu = 0$, these orthogonal functions form a complete set,

$$J_0 \left(x_{01} \frac{\rho}{a} \right), \quad J_0 \left(x_{02} \frac{\rho}{a} \right), \quad J_0 \left(x_{03} \frac{\rho}{a} \right), \ldots,$$

where x_{0n} are numerical values in Table 5.2. We plot these functions.

Worksheet 5.8 For essentially all problems requiring Bessel functions, we must find the roots, for which purpose we use the `fsolve` command to find the roots for $J_0(x)$. We first make a plot of $J_\nu(x)$, so that from the graph we can supply a range for `fsolve` to seek numerical solutions. We plot a set of orthogonal Bessel functions of zeroth order.

```
> plot(BesselJ(0,x), x=0..20);
```




```
> x0[1] := fsolve(BesselJ(0,x), x=2..3);
```

$$x0_1 := 2.404825558$$

```
> x0[2] := fsolve(BesselJ(0,x), x=5..6);
```

$$x0_2 := 5.520078110$$

```
> x0[3] := fsolve(BesselJ(0,x), x=8..9);
```

$$x0_3 := 8.653727913$$

```
> x0[4] := fsolve(BesselJ(0,x), x=11..12);
```

$$x0_4 := 11.79153444$$

```
> x0[5] := fsolve(BesselJ(0,x), x=14..15);
```

$$x0_5 := 14.93091771$$

```
> a := 1;
```

$$a := 1$$

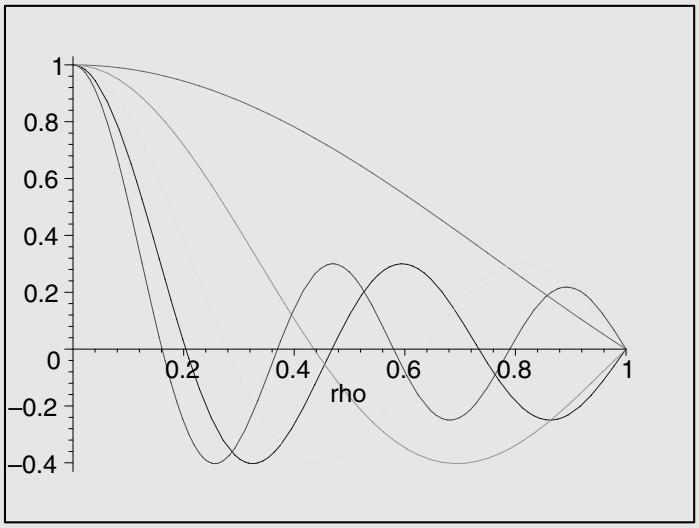
```
> N := 5:

> for n from 1 to N do

> k0[n] := x0[n]/a;

> end do:
```

```
> plot({seq(BesselJ(0, k0[n]*rho), n=1..5)}, rho=0..a);
```



We draw an analogy between Bessel functions and sine functions. In the Fourier series, the orthogonal functions are $\sin(kx)$, $\sin(2kx)$, $\sin(3kx)$, and so on; they are sine functions of which x is scaled by a factor of k, $2k$, $3k$, ... Similarly, for a Bessel function of the first kind and of zeroth order, we scale ρ by a factor of k_{01}, k_{02}, k_{03}, ..., where

$$k_{01} = \frac{x_{01}}{a}, \quad k_{02} = \frac{x_{02}}{a}, \quad k_{03} = \frac{x_{03}}{a}, \ldots .$$

For sine functions, such scaling makes $\sin(mkL) = 0$; for Bessel functions, $J_0(k_{0n}a) = 0$.

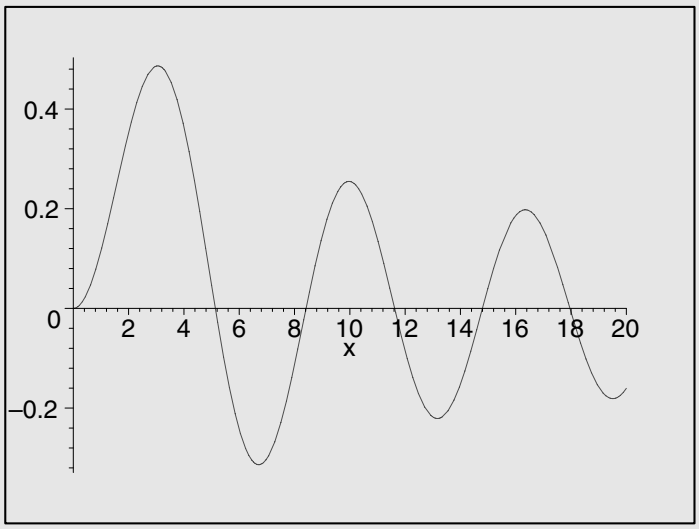
As another example, if $\nu = 2$, the orthogonal functions are

$$J_2\left(x_{21}\frac{\rho}{a}\right), \quad J_2\left(x_{22}\frac{\rho}{a}\right), \quad J_2\left(x_{23}\frac{\rho}{a}\right), \ldots .$$

We plot these functions also; again we must first evaluate the roots of $J_2(x)$.

Worksheet 5.9 Knowing the principle of numerical solution for the roots of the Bessel function, from now on we employ the `BesselJZeros(nu, n)` command to find the roots. The first argument `nu` is the order of the Bessel function, and the second argument `n` is the nth root of the Bessel function. This worksheet is almost identical to the preceding one except that we use $J_2(x)$.

```
> plot(BesselJ(2,x), x=0..20);
```




```
> x2[1] := evalf(BesselJZeros(2,1));
```

$$x2_1 := 5.135622302$$

```
> x2[2] := evalf(BesselJZeros(2,2));
```

$$x2_2 := 8.417244140$$

```
> x2[3] := evalf(BesselJZeros(2,3));
```

$$x2_3 := 11.61984117$$

```
> x2[4] := evalf(BesselJZeros(2,4));
```

$$x2_4 := 14.79595178$$

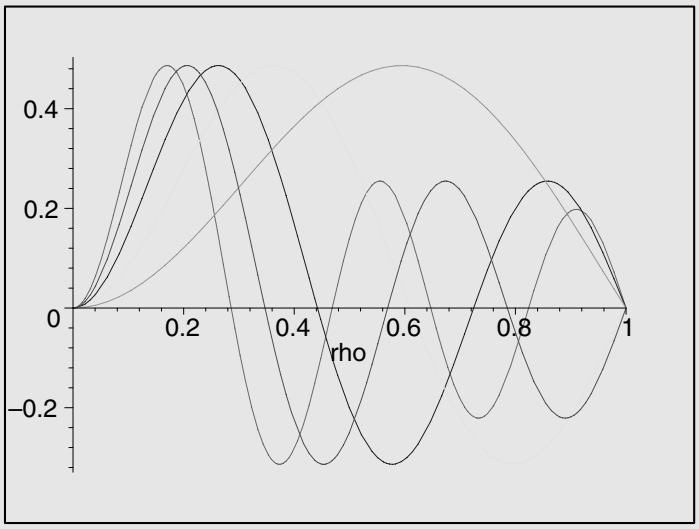
```
> x2[5] := evalf(BesselJZeros(2,5));
```

$$x2_5 := 17.95981949$$

```
> a := 1;
```

$$a := 1$$

```
> N := 5:
> for n from 1 to N do
> k2[n] := x2[n]/a;
> end do:
> plot({seq(BesselJ(2, k2[n]*rho), n=1..5)}, rho=0..a);
```



Because Bessel functions satisfy the orthogonality and completeness conditions, we can expand an arbitrary function of ρ on an interval $0 \leq \rho \leq a$ in a Fourier–Bessel series,

$$u(\rho) = \sum_{n=1}^{\infty} A_{\nu n} J_\nu \left(x_{\nu n} \frac{\rho}{a} \right), \tag{5.31}$$

or explicitly,

$$u(\rho) = A_{\nu 1} J_\nu \left(x_{\nu 1} \frac{\rho}{a} \right) + A_{\nu 2} J_\nu \left(x_{\nu 2} \frac{\rho}{a} \right) + A_{\nu 3} J_\nu \left(x_{\nu 3} \frac{\rho}{a} \right) + \ldots, \tag{5.31$'$}$$

where ν is fixed; the summation is over index n, the label for the nth root of this Bessel function. The coefficient is evaluated as[1]

$$A_{\nu n} = \frac{2}{a^2 J_{\nu+1}^2 (x_{\nu n})} \int_0^a \rho u(\rho) J_\nu \left(x_{\nu n} \frac{\rho}{a} \right) d\rho. \tag{5.32}$$

Be aware of an extra term ρ present as a weight function.

Example 5.5 Expand a function

$$u(\rho) = 1, \quad 0 < \rho < 1, \tag{5.33}$$

in the Fourier–Bessel series using Bessel functions of the first kind and of order zero.

[1] Jackson 1999, p. 115.

Solution For this problem, $a = 1$, we must evaluate roots x_{0n} such that $J_0(x_{0n}) = 0$. These roots are listed in Table 5.2, which contains values derived by a numerical method. From equation (5.32),

$$A_{01} = \frac{2}{J_1^2(x_{01})} \int_0^1 \rho J_0\left(x_{01}\rho\right) d\rho = 1.602, \quad (x_{01} = 2.405),$$

$$A_{02} = \frac{2}{J_1^2(x_{02})} \int_0^1 \rho J_0\left(x_{02}\rho\right) d\rho = -1.065, \quad (x_{02} = 5.520),$$

$$A_{03} = \frac{2}{J_1^2(x_{03})} \int_0^1 \rho J_0\left(x_{03}\rho\right) d\rho = 0.851, \quad (x_{03} = 8.654),$$

and so on. Thus we have

$$u(\rho) = 1.602J_0(2.405\rho) - 1.062J_0(5.520\rho) + 0.851J_0(8.654\rho) + \ldots.$$

Worksheet 5.10 Evaluation of coefficients for the Fourier–Bessel series has exactly the same formalism as that for the Fourier series: instead of `sin`, we use `BesselJ`, remembering to insert the weight function ρ. To perform repeated integrations we naturally employ a `for` loop.

```
> x0[1] := evalf(BesselJZeros(0,1));
```
$$x0_1 := 2.404825558$$
```
> x0[2] := evalf(BesselJZeros(0,2));
```
$$x0_2 := 5.520078110$$
```
> x0[3] := evalf(BesselJZeros(0,3));
```
$$x0_3 := 8.653727913$$
```
> x0[4] := evalf(BesselJZeros(0,4));
```
$$x0_4 := 11.79153444$$
```
> x0[5] := evalf(BesselJZeros(0,5));
```
$$x0_5 := 14.93091771$$
```
> x0[6] := evalf(BesselJZeros(0,6));
```
$$x0_6 := 18.07106397$$
```
> x0[7] := evalf(BesselJZeros(0,7));
```
$$x0_7 := 21.21163663$$
```
> x0[8] := evalf(BesselJZeros(0,8));
```
$$x0_8 := 24.35247153$$
```
> x0[9] := evalf(BesselJZeros(0,9));
```
$$x0_9 := 27.49347913$$
```
> x0[10] := evalf(BesselJZeros(0,10));
```
$$x0_{10} := 30.63460647$$

```
> x0[11] := evalf(BesselJZeros(0,11));
```

$$x0_{11} := 33.77582021$$

```
> a := 1;
```

$$a := 1$$

```
> N := 11:

> for n from 1 to N do

> k0[n] := x0[n]/a;

> end do:

> for n from 1 to N do
> A0[n] :=
> 2/(a^2*BesselJ(1,k0[n]*a)^2)*int(rho*BesselJ(0,k0[n]*rho),
> rho=0..a);

> end do;
```

$$A0_1 := 1.601974698$$
$$A0_2 := -1.064799258$$
$$A0_3 := 0.8513991924$$
$$A0_4 := -0.7296452398$$
$$A0_5 := 0.6485236140$$
$$A0_6 := -0.5895428294$$
$$A0_7 := 0.5441801960$$
$$A0_8 := -0.5078936308$$
$$A0_9 := 0.4780124976$$
$$A0_{10} := -0.4528505588$$
$$A0_{11} := 0.4312838768$$

```
> f := m -> add(A0[n]*BesselJ(0,k0[n]*rho), n=1..m);
```

$$f := m \to \mathrm{add}(A0_n\,\mathrm{BesselJ}(0,\, k0_n\,\rho),\, n = 1..m)$$

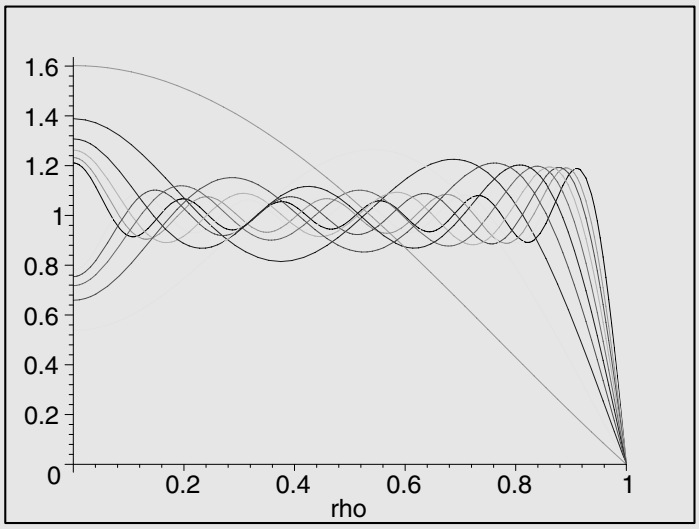
```
> with(plots):
```

```
Warning, the name changecoords has been redefined
```

```
> p1 := plot({seq(f(m), m=1..N-1)}, rho=0..a):

> p2 := plot(f(N), rho=0..a, thickness=2, color=black):

> display([p1, p2]);
```



We plot the progressive improvement of the representation as N increases.

Example 5.6 Expand a function

$$u(\rho) = \rho(1-\rho), \quad 0 < \rho < 1, \tag{5.34}$$

in the Fourier–Bessel series using Bessel functions of the first kind of order two.

Solution In this problem, $a = 1$; we require roots x_{2n} such that $J_2(x_{2n}) = 0$. From equation (5.32),

$$A_{2n} = \frac{2}{J_3^2(x_{0n})} \int_0^1 \rho[\rho(1-\rho)] J_2\left(x_{0n}\rho\right) d\rho,$$

we obtain

$$u(\rho) = 0.527 J_2(5.136\rho) + 0.098 J_2(8.417\rho) + 0.876 J_2(11.620\rho) + \ldots.$$

Worksheet 5.11 This approach is exactly the same as in the preceding worksheet, except that orthogonal functions are Bessel functions of order two, `BesselJ(2,x)`.

```
> x2[1] := evalf(BesselJZeros(2,1));
```

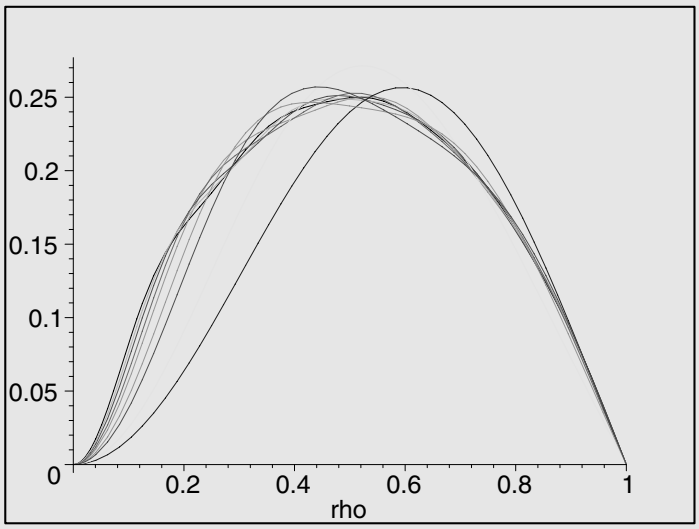
$$x2_1 := 5.135622302$$

```
> x2[2] := evalf(BesselJZeros(2,2));
```

$$x2_2 := 8.417244140$$

```
> x2[3] := evalf(BesselJZeros(2,3));
```
$$x2_3 := 11.61984117$$
```
> x2[4] := evalf(BesselJZeros(2,4));
```
$$x2_4 := 14.79595178$$
```
> x2[5] := evalf(BesselJZeros(2,5));
```
$$x2_5 := 17.95981949$$
```
> x2[6] := evalf(BesselJZeros(2,6));
```
$$x2_6 := 21.11699705$$
```
> x2[7] := evalf(BesselJZeros(2,7));
```
$$x2_7 := 24.27011231$$
```
> x2[8] := evalf(BesselJZeros(2,8));
```
$$x2_8 := 27.42057355$$
```
> x2[9] := evalf(BesselJZeros(2,9));
```
$$x2_9 := 30.56920450$$
```
> a := 1;
```
$$a := 1$$
```
> N := 9:
> for n from 1 to N do
> k2[n] := x2[n]/a;
> end do:
> for n from 1 to N do
> A2[n] :=
> 2/(a^2*BesselJ(3,k2[n]*a)^2)*int(rho*rho*(1-rho)
> *BesselJ(2,k2[n]*rho), rho=0..a);
> end do;
```
$$A2_1 := 0.5273837770$$
$$A2_2 := 0.09805457534$$
$$A2_3 := 0.08758732210$$
$$A2_4 := 0.03433336328$$
$$A2_5 := 0.03495744094$$
$$A2_6 := 0.01752244388$$
$$A2_7 := 0.01865994794$$
$$A2_8 := 0.01064622619$$
$$A2_9 := 0.01156746695$$
```
> f := m -> add(A2[n]*BesselJ(2,k2[n]*rho), n=1..m);
```
$$f := m \to \mathrm{add}(A2_n\,\mathrm{BesselJ}(2,\ k2_n\,\rho),\ n = 1..m)$$
```
> with(plots):
```

```
Warning, the name changecoords has been redefined
> p1 := plot({seq(f(m), m=1..N-1)}, rho=0..a):
> p2 := plot(f(N), rho=0..a, thickness=2, color=black):
> display([p1, p2]);
```



5.6 Summary of Special Functions

A complete set of orthogonal functions serve as a basis for expansion to represent most functions of interest in physics. Such an expansion is written in equation (5.18),

$$u(x) = \sum_{n=1}^{\infty} c_n f_n(x),$$

and coefficients are evaluated according to equation (5.19),

$$c_n = \int_a^b f_n^*(x) w(x) u(x) dx,$$

where $w(x)$ is the weight function.

Most students are familiar with the Fourier series, an expansion in sinusoidal functions, but fewer students are acquainted with expansion in special functions such as Bessel functions. One reason might be that some students feel alien to these special functions. The procedure to expand a function in a complete set of orthogonal functions, such as Legendre polynomials or

Bessel functions, is identical to that for sinusoidal functions, and Maple is extremely useful in the performance of this task because it eliminates the manual calculation of integrals.

Legendre polynomials are solutions of a second-order differential equation, which belongs to the Sturm–Liouville system. In addition to Legendre polynomials, there are Hermite polynomials and Laguerre polynomials, which are important in quantum mechanics. We postpone discussion of these orthogonal polynomials until Chapters 15 and 16, but here follows a summary.

- sines
  differential equation:

$$\frac{d^2 f_n}{dx^2} + n^2 f_n = 0 \tag{5.35}$$

  solution: $f_n = \sin(nx)$; Maple command: `sin(n*x)`
  expansion $(-\pi < x < \pi)$ for an odd function $u(x) = -u(-x)$:

$$u(x) = \sum_{n=1}^{\infty} c_n \sin(nx) \tag{5.36}$$

  coefficients:

$$c_n = \frac{1}{\pi} \int_{-\pi}^{\pi} \sin(nx) u(x) dx \tag{5.37}$$

- Legendre polynomials
  differential equation:

$$(1 - x^2) \frac{d^2 P_l}{dx^2} - 2x \frac{dP_l}{dx} + l(l+1) P_l = 0 \tag{5.38}$$

  solution: $P_l(x)$; Maple command: `LegendreP(l, x)`
  expansion $(-1 < x < 1)$:

$$u(x) = \sum_{l=0}^{\infty} c_l P_l(x) \tag{5.39}$$

  coefficients:

$$c_l = \frac{2l+1}{2} \int_{-1}^{1} P_l(x) u(x) dx \tag{5.40}$$

- Bessel functions
  differential equation:

$$\rho^2 \frac{d^2 J_\nu}{d\rho^2} + \rho \frac{dJ_\nu}{d\rho} + (\rho^2 - \nu^2) J_\nu = 0 \tag{5.41}$$

solution: $J_\nu(\rho)$; Maple command: `BesselJ(nu, rho)`
expansion $(0 < x < a)$ for a fixed ν:

$$u(\rho) = \sum_{n=1}^{\infty} A_{\nu n} J_\nu \left(x_{\nu n} \frac{\rho}{a} \right) \tag{5.42}$$

where $x_{\nu n}$ are numerical values listed in Table 5.2; the index of summation is n, the nth roots of $J_\nu(x)$.
coefficients:

$$A_{\nu n} = \frac{2}{a^2 J_{\nu+1}^2(x_{\nu n})} \int_0^a \rho u(\rho) J_\nu \left(x_{\nu n} \frac{\rho}{a} \right) d\rho \tag{5.43}$$

This integral contains a weight function ρ.

- Hermite polynomials
differential equation:

$$\frac{d^2 H_n}{dx^2} - 2x \frac{dH_n}{dx} + 2nH_n = 0 \tag{5.44}$$

solution: $H_n(x)$; Maple command: `HermiteH(n, x)`
Further discussion arises in relation to a quantum oscillator.

- Laguerre polynomials
differential equation:

$$x \frac{d^2 L_n}{dx^2} + (1 - x) \frac{dL_n}{dx} + nL_n = 0 \tag{5.45}$$

solution: $L_n(x)$; Maple command: `LaguerreL(n, x)`
Further discussion arises in relation to the radial equation for the hydrogen atom.

Exercises

1. Calculate the Fourier transform $\alpha(k)$ of a function

$$u(x) = \begin{cases} 0 & x < 0 \\ xe^{-x} & x > 0 \end{cases},$$

then perform the inverse Fourier transformation on $\alpha(k)$. Plot this function, and compare with $u(x)$.

2. Calculate the Fourier transform $\alpha(k)$ of the Gaussian function

$$u(x) = \frac{1}{\sqrt{2\pi}a} e^{-\frac{x^2}{2a^2}}, \tag{5.46}$$

then plot the Gaussian function and its Fourier transform for various a.

3. A function $u(x)$ and its Fourier transform $\alpha(k)$ satisfy the Fourier–Parseval identity:

$$\int_{-\infty}^{\infty} |u(x)|^2 \, dx = \int_{-\infty}^{\infty} |\alpha(k)|^2 dk. \tag{5.47}$$

Check whether this theorem holds for the example in Section 5.2 by comparing the integrals

$$\int_{-1/2}^{1/2} 1^2 \, dx$$

and

$$\int_{-\infty}^{\infty} \left(\sqrt{\frac{2}{\pi}} \frac{\sin \frac{k}{2}}{k} \right)^2 dk.$$

Try also the Gaussian function and its Fourier transform in the preceding exercise.

4. Expand this function,

$$u(x) = \sin(x), \quad -1 < x < 1,$$

defined on an interval $-1 < x < 1$, in Legendre polynomials. Make a plot to compare the series and the original function.

5. Expand this function,

$$u(\rho) = \sin(\rho), \quad 0 < \rho < 1,$$

defined on an interval $0 < \rho < 1$, in Bessel functions of the first kind of order 4, $J_4(\rho)$. Make a plot to compare the series and the original function.

6. Expand this function on an interval $0 < x < 6$,

$$u(x) = \begin{cases} 0, & 0 < x < 1, \\ x - 1, & 1 < x < 2, \\ 1, & 2 < x < 3, \\ -1, & 3 < x < 4, \\ x - 5, & 4 < x < 5, \\ 0, & 5 < x < 6, \end{cases}$$

in

(a) a Fourier series,

(b) a Bessel function of the first kind of order 0, $J_0(x)$,

(c) a Bessel function of the first kind of order 1, $J_1(x)$,

(d) a Bessel function of the first kind of order 2, $J_2(x)$.

Produce a graph for each expansion to observe the accuracy of the approximation.

7. Use Rodrigues' formula in equation (5.27) to generate the first five Legendre polynomials.

8. The generating function for the Hermite polynomials $H_n(x)$ is

$$\psi(x,t) = e^{-t^2+2tx},$$

such that

$$\sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n = e^{-t^2+2tx}. \tag{5.48}$$

Use the `taylor` command to generate the first five Hermite polynomials, and compare the result with `HermiteH`.

9. The generating function for the Laguerre polynomials $L_n(x)$ is

$$\psi(x,t) = \frac{e^{-xt/(1-t)}}{1-t},$$

such that

$$\sum_{n=0}^{\infty} \frac{L_n(x)}{n!} t^n = \frac{e^{-xt/(1-t)}}{1-t}. \tag{5.49}$$

Use the `taylor` command to generate the first five Laguerre polynomials, and compare the result with `LaguerreL`.

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6 Electrostatics

In this chapter we introduce electrostatics. An electric field can be calculated by Coulomb's law, which generally requires sophisticated calculations such as elliptic integrals. Maple is suitable and convenient for undertaking this type of task, especially in those situations when curvilinear coordinates are preferable. Because electric and magnetic fields are vectors, we carefully examine their meaning and representation in the context of symbolic computation.

6.1 Coulomb's Law

Two stationary electric charges q_1 and q_2 attract or repel each other with a force directly proportional to the product of the charges and inversely proportional to the square of the distance r_{12} between them,

$$\mathbf{F}_1 = \frac{1}{4\pi\epsilon_0}\frac{q_1 q_2}{r_{12}^2}\,\mathbf{e}_{12} = -\mathbf{F}_2, \tag{6.1}$$

where $\mathbf{e}_{12}$ is the normalized vector from q_2 to q_1; we will discuss this vector in detail below. This is Coulomb's law, which is based on experiment.

In SI units, the force is measured in newtons (N), distance in meters (m), and charge in coulombs (C). The constant ϵ_0 is called the permittivity of free space:

$$\epsilon_0 = 8.854187817\ldots \times 10^{-12}\ \mathrm{C}^2\,\mathrm{N}^{-1}\,\mathrm{m}^{-2}. \tag{6.2}$$

We separate the equation of the force between electric charges in two factors by defining an electric field $\mathbf{E}$:

$$\mathbf{F}_1 = q_1\mathbf{E}, \quad \mathbf{E} = \frac{1}{4\pi\epsilon_0}\frac{q_2}{r_{12}^2}\,\mathbf{e}_{12}. \tag{6.3}$$

Although the electric field seems merely an artifice of algebraic rearrangement, we encourage the reader to regard the field itself as a fundamental quantity of physical reality. A charged particle q in the presence of an electric field $\mathbf{E}$ experiences a force $\mathbf{F}_\mathrm{e} = q\mathbf{E}$; this formula is analogous to $\mathbf{F}_\mathrm{g} = m\mathbf{g}$, which describes the force acting on a particle of mass m in the presence of a gravitational field $\mathbf{g}$. The main objective of this and the next chapter is to find the electric field.

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Electromagnetism has a linear structure, therefore electric fields satisfy the principle of superposition. For charge as a continuous distribution, electric field is calculated from this integral:

$$\mathbf{E}(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}_2)}{r_{12}^2}\, \mathbf{e}_{12}\, d\tau_2. \tag{6.4}$$

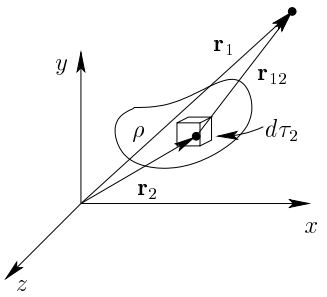


Figure 6.1: Notation for Coulomb's law.

The importance of notation in this equation cannot be emphasized too much: once one understands this notation, one can readily proceed with calculations that Maple can directly perform. Referring to Figure 6.1, we define $\mathbf{r}_1$ as the position vector of the *field point*, at which we intend to measure the strength of the field, and $\mathbf{r}_2$ as the position vector of the *source point*, at which the charge element contributes to the field. The *separation vector* from $\mathbf{r}_1$ to $\mathbf{r}_2$ is

$$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2, \quad r_{12} = |\mathbf{r}_{12}|. \tag{6.5}$$

We use the unbold symbol r_{12} to denote the length of the separation vector. The unit vector $\mathbf{e}_{12}$ is the normalized separation vector,

$$\mathbf{e}_{12} = \frac{\mathbf{r}_{12}}{r_{12}}, \tag{6.6}$$

which also indicates the direction of the electric field contributed by a charge element at $\mathbf{r}_2$. Integration is performed in the space of the source, $\mathbf{r}_2$, for which $d\tau_2$ denotes the volume element. We obtain the electric field as a function of $\mathbf{r}_1$.

If we are given the surface charge density, $\sigma(\mathbf{r}_2)$, we express the integral as

$$\mathbf{E}(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0} \int \frac{\sigma(\mathbf{r}_2)}{r_{12}^2}\, \mathbf{e}_{12}\, da_2, \tag{6.7}$$

with da_2 as the area element. Similarly, if we are given the line charge density, $\lambda(\mathbf{r}_2)$, the integral is

$$\mathbf{E}(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0} \int \frac{\lambda(\mathbf{r}_2)}{r_{12}^2}\, \mathbf{e}_{12}\, dl_2, \tag{6.8}$$

with dl_2 as the line element.

Example 6.1 Find the electric field at a distance z above one end of a segment of a straight line of length L that carries a uniform line charge λ. This problem is similar to one in Griffiths 1999, p. 63, problem 2.3 (see Bibliography).

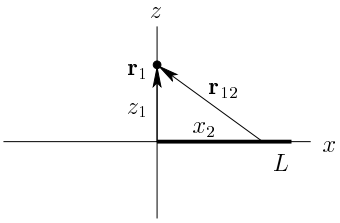


Figure 6.2: Electric field due to a charged wire.

Solution According to Figure 6.2, the field point is situated on the z axis, whereas the source points lie on the x axis. We express these conditions as

$$\mathbf{r}_1 = z_1\hat{\mathbf{z}}, \quad \mathbf{r}_2 = x_2\hat{\mathbf{x}}.$$

Directly following these definitions, we find the separation vector and its length,

$$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2, \quad r_{12} = \sqrt{x_2^2 + z_1^2},$$

and the normalized separation vector and line element,

$$\mathbf{e}_{12} = \frac{-x_2}{\sqrt{x_2^2 + z_1^2}}\hat{\mathbf{x}} + \frac{z_1}{\sqrt{x_2^2 + z_1^2}}\hat{\mathbf{z}}, \quad dl_2 = dx_2.$$

Having all the ingredients required for the application of Coulomb's law, we proceed to evaluate the integrals,

$$E_x = \frac{1}{4\pi\epsilon_0}\int_0^L \frac{\lambda}{x_2^2 + z_1^2}\frac{-x_2}{\sqrt{x_2^2 + z_1^2}}\,dx_2 = \frac{1}{4\pi\epsilon_0}\frac{\lambda(|z_1| - \sqrt{L^2 + z_1^2})}{|z_1|\sqrt{L^2 + z_1^2}}, \tag{6.9}$$

and

$$E_z = \frac{1}{4\pi\epsilon_0}\int_0^L \frac{\lambda}{x_2^2 + z_1^2}\frac{z_1}{\sqrt{x_2^2 + z_1^2}}\,dx_2 = \frac{1}{4\pi\epsilon_0}\frac{\lambda L}{z_1\sqrt{L^2 + z_1^2}}. \tag{6.10}$$

Once we are clear about various vectors, it is straightforward to use Maple to perform the calculations.

Worksheet 6.1 We use the `LinearAlgebra` package, which enables almost all operations on vectors. To find the length of a vector, which is officially known as the 2-norm, we employ Maple's command `Norm(r12, 2)`. The unit vector $\mathbf{e}_{12}$ is found using the `Normalize` command. Because Maple inherently assumes every parameter to be complex, we employ the `assume` command to inform Maple that physical quantities such as x_2 and z_1 are real. Finally, we apply the `int` command to evaluate the integrals.

```
> assume(x2, real, z1, real):
> with(LinearAlgebra):
> r2vec := < x2 | 0 | 0 >;
```

$$r2vec := [x2,\ 0,\ 0]$$

```
> r1vec := < 0 | 0 | z1 >;
```

$$r1vec := [0,\ 0,\ z1]$$

```
> r12vec := r1vec - r2vec;
```

$$r12vec := [-x2,\ 0,\ z1]$$

```
> e12 := Normalize(r12vec, 2):
> e12 := map(simplify, e12);
```

$$e12 := \left[-\frac{x2}{\sqrt{x2^2 + z1^2}},\ 0,\ \frac{z1}{\sqrt{x2^2 + z1^2}}\right]$$

```
> r12 := Norm(r12vec, 2):
> r12 := simplify(r12);
```

$$r12 := \sqrt{x2^2 + z1^2}$$

```
> Ez := int(lambda*e12[3]/r12^2, x2=0..L);
```

$$Ez := \frac{\lambda\, L}{z1\, \sqrt{L^2 + z1^2}}$$

```
> Ex := int(lambda*e12[1]/r12^2, x2=0..L):
> Ex := simplify(Ex);
```

$$Ex := \frac{\lambda \left(|z1| - \sqrt{L^2 + z1^2}\right)}{\sqrt{L^2 + z1^2}\ |z1|}$$

6.2 Curvilinear Coordinates

In some problems, the use of spherical or cylindrical coordinates greatly simplifies the calculations. When we undertake vector calculus in curvilinear coordinates, complications arise. It is worthwhile clarifying some concepts.

In elementary courses, a vector is conceived as a directed line segment, or a quantity with both a magnitude and a direction, such as the position vectors in Figure 6.1. In modern mathematics, a vector itself has a meaning independent of coordinates, and we can perform vector operations – addition, scalar multiplication, dot-product, and cross-product – in abstract form, without reference to any particular coordinate system. The reason for introducing coordinates is that we can resolve a vector into components, which are numbers (or symbols for them)

so that it is easier to compute with our brain or a computer. Newton's second law $\mathbf{F} = m\ddot{\mathbf{r}}$, and Maxwell's equations, as we will later learn, are independent of the choice of coordinates. Abstraction of vectors is elegant, but it is more practical to analyze vectors in components using symbolic computation software.

In three dimensions, one can express a vector $\mathbf{A}$ as a linear combination of any three non-coplanar vectors, such as $\mathbf{V}_1$, $\mathbf{V}_2$ and $\mathbf{V}_3$ in a relation

$$\mathbf{A} = \alpha\mathbf{V}_1 + \beta\mathbf{V}_2 + \gamma\mathbf{V}_3, \tag{6.11}$$

where the coefficients α, β and γ are scalar quantities. The most common choice of these three vectors is the Cartesian basis, consisting of three unit vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ parallel to the x, y and z axes, respectively. We can express any arbitrary vector $\mathbf{A}$ in terms of these basis vectors,

$$\mathbf{A} = A_x\hat{\mathbf{x}} + A_y\hat{\mathbf{y}} + A_z\hat{\mathbf{z}};$$

coefficients A_x, A_y and A_z constitute the components of $\mathbf{A}$. A vector expressed in the above form, called the basis format, contains both *components* and *basis vectors*. Comparing components of Newton's second law in each individual basis vector, we obtain $F_x = m\ddot{x}$, and $F_y = m\ddot{y}$, which is the method we used to treat the projectile motion in Section 1.5.

When we add two vectors, we write

$$\mathbf{A} + \mathbf{B};$$

this sum exists without reference to coordinates. We can resolve this sum of two vectors, and to do so in Cartesian coordinates is simple,

$$\mathbf{A} + \mathbf{B} = (A_x + B_x)\hat{\mathbf{x}} + (A_y + B_x)\hat{\mathbf{y}} + (A_z + B_z)\hat{\mathbf{z}}.$$

An alternative way to write a vector $\mathbf{A}$ is to use spherical coordinates; according to this system, the basis vectors are $\hat{\mathbf{r}}$, $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$, which are tangent to r, θ and ϕ, respectively. We express such a vector as

$$\mathbf{A} = A_r\hat{\mathbf{r}} + A_\theta\hat{\boldsymbol{\theta}} + A_\phi\hat{\boldsymbol{\phi}},$$

but we cannot calculate a sum of two arbitrary vectors in the same way as we did with the Cartesian basis. For instance, there is no such thing as

$$\mathbf{A} + \mathbf{B} = (A_r + B_r)\hat{\mathbf{r}} + (A_\theta + B_\theta)\hat{\boldsymbol{\theta}} + (A_\phi + B_\phi)\hat{\boldsymbol{\phi}}, \qquad \text{wrong!}$$

because $\hat{\mathbf{r}}$ depends on position. A cumbersome notation $\hat{\mathbf{r}}(\theta, \phi)$ is more accurate, as do the other two basis vectors. This instance demonstrates that one should not blindly apply properties of Cartesian vectors to vectors in a curvilinear system, particularly when one calculates the separation vector $\mathbf{r}_{12}$.

Another serious problem arises when we undertake vector calculus in curvilinear coordinates. When we perform differentiation on a vector, we must also differentiate with respect to basis

vectors. The radial component of Newton's second law in spherical coordinates is *not* $F_r = m\ddot{r}$, but $F_r = m(\ddot{r} - r\dot{\theta}^2)$. Similarly, when we evaluate an integral of a vector, the basis vectors might also depend on position. With these deceiving examples, we alert the reader to treat curvilinear coordinates with great care.

Examining equation (6.4), we discern that there are actually three integrals, and the integrand of each contains the basis vector. *Only* in Cartesian coordinates can we write the electric field as

$$\mathbf{E} = E_x\hat{\mathbf{x}} + E_y\hat{\mathbf{y}} + E_z\hat{\mathbf{z}}, \tag{6.12}$$

with components

$$E_x = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(\mathbf{r}_2)}{r_{12}^2}\,(\mathbf{e}_{12})_x\,d\tau_2, \tag{6.13a}$$

$$E_y = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(\mathbf{r}_2)}{r_{12}^2}\,(\mathbf{e}_{12})_y\,d\tau_2, \tag{6.13b}$$

$$E_z = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(\mathbf{r}_2)}{r_{12}^2}\,(\mathbf{e}_{12})_z\,d\tau_2, \tag{6.13c}$$

where $(\mathbf{e}_{12})_x$ is the x component of $\mathbf{e}_{12}$, etc. We can write the integrals in this form because the Cartesian basis vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ do not depend on position, so that we can remove them from the integral. In general, a basis of curvilinear coordinates depends on coordinates, which must remain inside the integral.

Because we are familiar with the properties of Cartesian coordinates, and because we seek to avoid any undesired complication when integrating a basis of curvilinear coordinates, for most tasks it is safer to write the integral using equations (6.12) and (6.13). Our discretion by using the Cartesian basis does not prevent us from taking advantage of curvilinear coordinates: integrands in three elementary integrals in equation (6.13) can be expressed in curvilinear coordinates, which simply involves a change of variables. We illustrate our approach with examples.

6.2.1 Spherical Coordinates

We can apply spherical coordinates to express a vector but still use the Cartesian basis; we describe it clumsily as a vector in the Cartesian basis with spherical coordinates. In this system,

$$\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} = r\sin\theta\cos\phi\,\hat{\mathbf{x}} + r\sin\theta\sin\phi\,\hat{\mathbf{y}} + r\cos\theta\,\hat{\mathbf{z}}. \tag{6.14}$$

We can genuinely view this as a change of variables. The notation

$$[r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta]$$

commonly serves to express a vector, which resembles the expression in Maple. As we have mentioned earlier that a vector resolved in a particular coordinate system has both components and basis vectors, one must be aware what the basis vectors are for those three components. In this chapter we make efforts to explicitly express both the components and the basis vectors.

Differential elements are necessary when we perform integration. The infinitesimal displacement in spherical coordinates is

$$d\mathbf{l} = dr\,\hat{\mathbf{r}} + rd\theta\,\hat{\boldsymbol{\theta}} + r\sin\theta d\phi\,\hat{\boldsymbol{\phi}}. \tag{6.15}$$

The infinitesimal volume element in spherical coordinates is

$$d\tau = r^2\,\sin\theta\,dr\,d\theta\,d\phi. \tag{6.16}$$

There is no unique way to specify the infinitesimal area element in spherical coordinates,

$$d\mathbf{a} = \begin{cases} r^2\sin\theta\,d\theta\,d\phi\,\hat{\mathbf{r}} \\ r\sin\theta\,dr\,d\phi\,\hat{\boldsymbol{\theta}} \\ rdr\,d\theta\,\hat{\boldsymbol{\phi}}, \end{cases} \tag{6.17}$$

because they depend on orientation.

Unit basis vectors in spherical coordinates are related to those in Cartesian coordinates by these relations,

$$\begin{aligned} \hat{\mathbf{x}} &= \sin\theta\,\cos\phi\,\hat{\mathbf{r}} + \cos\theta\,\cos\phi\,\hat{\boldsymbol{\theta}} - \sin\phi\,\hat{\boldsymbol{\phi}}, \\ \hat{\mathbf{y}} &= \sin\theta\,\sin\phi\,\hat{\mathbf{r}} + \cos\theta\,\sin\phi\,\hat{\boldsymbol{\theta}} + \cos\phi\,\hat{\boldsymbol{\phi}}, \\ \hat{\mathbf{z}} &= \cos\theta\,\hat{\mathbf{r}} - \sin\theta\,\hat{\boldsymbol{\theta}}, \end{aligned} \tag{6.18}$$

which are useful if we intend to express a vector in the spherical basis; note that the transformation depends on position through θ and ϕ.

Example 6.2 A sphere of radius R carries a uniform volume charge density ρ. Calculate the electric field a distance z from the center of the sphere; treat the cases $z < R$ and $z > R$. Express the answers in terms of total charge Q on the sphere.

Solution The volume charge density is

$$\rho = \frac{3Q}{4\pi R^3}.$$

Because of spherical symmetry of the source, we can choose the position vector for the field point at

$$\mathbf{r}_1 = z_1\hat{\mathbf{z}},$$

which is easier to calculate. It is advantageous to employ spherical coordinates with the Cartesian basis for the position vector for the source:

$$\mathbf{r}_2 = r_2\sin\theta_2\cos\phi_2\,\hat{\mathbf{x}} + r_2\sin\theta_2\sin\phi_2\,\hat{\mathbf{y}} + r_2\cos\theta_2\,\hat{\mathbf{z}}.$$

The separation vector in the Cartesian basis and its length directly follow:

$$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2, \quad r_{12} = \sqrt{r_2^2 + z_1^2 - 2r_2 z_1 \cos\theta_2},$$
$$\mathbf{e}_{12} = \frac{-r_2 \sin\theta_2 \cos\phi_2}{\sqrt{r_2^2 + z_1^2 - 2r_2 z_1 \cos\theta_2}}\hat{\mathbf{x}} + \frac{-r_2 \sin\theta_2 \sin\phi_2}{\sqrt{r_2^2 + z_1^2 - 2r_2 z_1 \cos\theta_2}}\hat{\mathbf{y}} + \frac{z_1 - r_2 \cos\theta_2}{\sqrt{r_2^2 + z_1^2 - 2r_2 z_1 \cos\theta_2}}\hat{\mathbf{z}}.$$

Each vector is in the Cartesian basis; we express x_2, y_2 and z_2 in terms of r_2, θ_2 and ϕ_2, so that it is convenient to set limits for integration. Because $(\mathbf{e}_{12})_x$ contains $\cos\phi_2$ and $(\mathbf{e}_{12})_y$ contains $\sin\phi_2$, the integral over a complete cycle of ϕ_2 is zero. To verify this fact, one simply invokes Maple to evaluate the integrals directly. The only nonvanishing term is E_z. For z_1 outside the sphere,

$$E_z = \frac{1}{4\pi\epsilon_0}\int_0^R dr_2 \int_0^\pi d\theta_2 \int_0^{2\pi} d\phi_2 \rho \frac{1}{r_2^2 + z_1^2 - 2r_2 z_1 \cos\theta_2} \frac{z_1 - r_2\cos\theta_2}{\sqrt{r_2^2 + z_1^2 - 2r_2 z_1 \cos\theta_2}} r_2^2 \sin\theta_2 = \frac{Q}{4\pi\epsilon_0 z_1^2},$$

and for z_1 inside the sphere,

$$E_z = \frac{1}{4\pi\epsilon_0}\int_0^{z_1} dr_2 \int_0^\pi d\theta_2 \int_0^{2\pi} d\phi_2 \rho \frac{1}{r_2^2 + z_1^2 - 2r_2 z_1 \cos\theta_2} \frac{z_1 - r_2\cos\theta_2}{\sqrt{r_2^2 + z_1^2 - 2r_2 z_1 \cos\theta_2}} r_2^2 \sin\theta_2 = \frac{Q z_1}{4\pi\epsilon_0 R^3}.$$

Although these integrals appear complicated, Maple returns elegant results.

Worksheet 6.2 Directly according to the definition of Coulomb's law, denoting z_1 as `z1`, and r_2, θ_2 and ϕ_2 as `r2`, `theta2` and `phi2`, respectively, we form the integrals. We use the `assume` and `additionally` commands to indicate whether the field point is inside or outside the sphere. We list the outside case; for the inside case, delete the comment signs from the pertinent assumption and integral. Maple provides the `Normalize` and `Norm` commands to calculate $\mathbf{e}_{12}$ (symbol `e12`) and r_{12} (symbol `r12`) conveniently.

```
> with(LinearAlgebra):
> assume(z1>0, r2>0, theta2, real, phi2, real, R>0);
> additionally(z1>R); #z1>R case
> #additionally(z1<R); #z1<R case
> rho := Q/(4/3*Pi*R^3);
```

$$\rho := \frac{3\,Q}{4\,\pi\,R^3}$$

```
> x2 := r2*sin(theta2)*cos(phi2); y2 := r2*sin(theta2)*sin(phi2);
z2 := r2*cos(theta2);
```

$$x2 := r2\sin(\theta 2)\cos(\phi 2)$$

$$y2 := r2\sin(\theta 2)\sin(\phi 2)$$

$$z2 := r2\cos(\theta 2)$$

```
> r2vec := < x2 | y2 | z2 >;
```

$$r2vec := [r2\sin(\theta 2)\cos(\phi 2),\ r2\sin(\theta 2)\sin(\phi 2),\ r2\cos(\theta 2)]$$

```
> r1vec := < 0 | 0 | z1 >;
```

$$r1vec := [0,\ 0,\ z1]$$

```
> r12vec := r1vec - r2vec;
```

$$r12vec := [-r2\sin(\theta 2)\cos(\phi 2),\ -r2\sin(\theta 2)\sin(\phi 2),\ z1 - r2\cos(\theta 2)]$$

```
> e12 := Normalize(r12vec, 2):
> r12 := Norm(r12vec, 2):
> e12 := map(simplify, e12);
```

$$e12 := \left[-\frac{r2\sin(\theta 2)\cos(\phi 2)}{\sqrt{\%1}},\ -\frac{r2\sin(\theta 2)\sin(\phi 2)}{\sqrt{\%1}},\ -\frac{-z1 + r2\cos(\theta 2)}{\sqrt{\%1}}\right]$$

$$\%1 := r2^2 + z1^2 - 2\,z1\,r2\cos(\theta 2)$$

```
> r12 := simplify(r12);
```

$$r12 := \sqrt{r2^2 + z1^2 - 2\,z1\,r2\cos(\theta 2)}$$

```
> Ezang := 1/(4*Pi*epsilon[0])*
> int(int(rho*r2^2*sin(theta2)*e12[3]/r12^2, phi2=0..2*Pi),
> theta2=0..Pi);
```

$$Ezang := \frac{3}{8}\,\frac{r2^2\,Q\,(\sqrt{(r2 - z1)^2} - r2 + z1)}{\pi\,\varepsilon_0\,\sqrt{(r2 - z1)^2}\,R^3\,z1^2}$$

```
> Ez := int(Ezang, r2=0..R); #z1>R case
```

$$Ez := \frac{1}{4}\,\frac{Q}{\pi\,\varepsilon_0\,z1^2}$$

```
> #Ez := int(Ezang, r2=0..z1); #z1<R case
```

Because we use the Cartesian basis, we write the electric field in the basis form as $\mathbf{E} = E_z\hat{\mathbf{z}}$. To express the electric field in the spherical basis, from equation (6.18), we have $r = z_1$ and $\hat{\mathbf{z}} = \hat{\mathbf{r}}$ at $\theta = 0$, thus we write

$$\mathbf{E} = \begin{cases} \dfrac{Q}{4\pi\epsilon_0 r^2}\hat{\mathbf{r}}, & r > R, \\ \dfrac{Qr}{4\pi\epsilon_0 R^3}\hat{\mathbf{r}}, & r < R. \end{cases} \tag{6.19}$$

This fact is obvious from the consideration of symmetry, because we recognize that the field is in a radial direction.

6.2.2 Cylindrical Coordinates

The position vector in the Cartesian basis with cylindrical coordinates is expressed as

$$\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} = \rho\cos\phi\,\hat{\mathbf{x}} + \rho\sin\phi\,\hat{\mathbf{y}} + z\,\hat{\mathbf{z}}. \tag{6.20}$$

Take care not to confuse coordinate ρ with the charge density, which is conventionally denoted by a symbol $\rho(\mathbf{r}_2)$.

The infinitesimal displacement in cylindrical coordinates is

$$d\mathbf{l} = d\rho\,\hat{\boldsymbol{\rho}} + \rho d\phi\,\hat{\boldsymbol{\phi}} + dz\,\hat{\mathbf{z}}. \tag{6.21}$$

The infinitesimal volume element is

$$d\tau = \rho\,d\rho\,d\phi\,dz. \tag{6.22}$$

No expression for the infinitesimal area element in a unique form is practicable,

$$d\mathbf{a} = \begin{cases} \rho\,d\phi\,dz\,\hat{\boldsymbol{\rho}} \\ d\rho\,dz\,\hat{\boldsymbol{\phi}} \\ \rho\,d\phi\,d\rho\,\hat{\mathbf{z}}, \end{cases} \tag{6.23}$$

because it depends on the orientation.

Unit basis vectors in cylindrical coordinates are related to those in Cartesian coordinates by these relations:

$$\begin{aligned} \hat{\mathbf{x}} &= \cos\phi\,\hat{\boldsymbol{\rho}} - \sin\phi\,\hat{\boldsymbol{\phi}}, \\ \hat{\mathbf{y}} &= \sin\phi\,\hat{\boldsymbol{\rho}} + \cos\phi\,\hat{\boldsymbol{\phi}}, \\ \hat{\mathbf{z}} &= \hat{\mathbf{z}}. \end{aligned} \tag{6.24}$$

Example 6.3 Consider a uniformly charged cylinder of radius R and height h, with total charge Q; evaluate the electric field at a distance d from the center of the top of the cylinder.

Solution The volume charge density is

$$\frac{Q}{\pi R^2 h}.$$

Setting the origin at the center of the bottom of the cylinder, the position vector for the field point is

$$\mathbf{r}_1 = z_1\hat{\mathbf{z}};$$

in this problem writing the position vector for the source in cylindrical coordinates with the Cartesian basis is beneficial:

$$\mathbf{r}_2 = \rho_2\cos\phi_2\hat{\mathbf{x}} + \rho_2\sin\phi_2\hat{\mathbf{y}} + z_2\hat{\mathbf{z}}.$$

We evaluate the separation vector and its length in the customary manner:

$$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2, \quad r_{12} = \sqrt{\rho_2^2 + (z_1 - z_2)^2},$$

$$\mathbf{e}_{12} = \frac{-\rho_2\cos\phi_2}{\sqrt{\rho_2^2 + (z_1 - z_2)^2}}\hat{\mathbf{x}} + \frac{-\rho_2\sin\phi_2}{\sqrt{\rho_2^2 + (z_1 - z_2)^2}}\hat{\mathbf{y}} + \frac{z_1 - z_2}{\sqrt{\rho_2^2 + (z_1 - z_2)^2}}\hat{\mathbf{z}}.$$

Because $(\mathbf{e}_{12})_x$ contains $\cos\phi_2$ and $(\mathbf{e}_{12})_y$ contains $\sin\phi_2$, which makes the integral over a complete cycle of ϕ_2 zero, we need only to integrate the z component,

$$E_z = \frac{1}{4\pi\epsilon_0}\int_0^R d\rho_2\int_0^{2\pi} d\phi_2\int_0^h dz_2\frac{Q}{\pi R^2 h}\frac{1}{\rho_2^2 + (z_1 - z_2)^2}\frac{z_1 - z_2}{\sqrt{\rho_2^2 + (z_1 - z_2)^2}}\rho_2$$
$$= \frac{1}{2\pi\epsilon_0}\frac{Q}{R^2 h}\left[\sqrt{R^2 + (z_1 - h)^2} + h - \sqrt{R^2 + z_1^2}\right].$$

Worksheet 6.3 Symbols `z1`, `rho2`, `phi2` and `z2` denote z_1, ρ_2, ϕ_2 and z_2, respectively. The calculations are similar to those in the preceding worksheet.

```
> with(LinearAlgebra):
> assume(z1>0, rho2>0, phi2>0, z2>0, h>0, R>0);
> additionally(z1>z2);
> den := Q/(Pi*R^2*h);
```

$$den := \frac{Q}{\pi\, R^2\, h}$$

```
> r2vec := < rho2*cos(phi2) | rho2*sin(phi2) | z2 >;
```

$$r2vec := [\rho 2\cos(\phi 2),\ \rho 2\sin(\phi 2),\ z2]$$

```
> r1vec := < 0 | 0 | z1 >;
```

$$r1vec := [0,\ 0,\ z1]$$

```
> r12vec := r1vec - r2vec;
```

$$r12vec := [-\rho 2\cos(\phi 2),\ -\rho 2\sin(\phi 2),\ z1 - z2]$$

```
> e12 := Normalize(r12vec, 2):
> e12 := map(simplify, e12);
```

$$e12 := \left[-\frac{\rho 2\cos(\phi 2)}{\sqrt{\%1}},\ -\frac{\rho 2\sin(\phi 2)}{\sqrt{\%1}},\ \frac{z1 - z2}{\sqrt{\%1}}\right]$$

$$\%1 := \rho 2^2 + z1^2 - 2\,z1\,z2 + z2^2$$

```
> r12 := Norm(r12vec, 2):
> r12 := simplify(r12);
```

$$r12 := \sqrt{\rho 2^2 + z1^2 - 2\,z1\,z2 + z2^2}$$

```
> Ez := 1/(4*Pi*epsilon[0])*int(int(int(den*e12[3]*rho2/r12^2,
> phi2=0..2*Pi), rho2=0..R), z2=0..h);
```

$$Ez := \frac{1}{2}\,\frac{Q\,(h + \sqrt{R^2 + z1^2 - 2\,z1\,h + h^2} - \sqrt{R^2 + z1^2})}{\pi\,\varepsilon_0\,R^2\,h}$$

6.3 Differential Vector Calculus

In this section we introduce the differential operator ∇ of vector calculus. In Cartesian coordinates, the gradient of a scalar function V, or a *scalar field*, is

$$\nabla V = \frac{\partial V}{\partial x}\hat{\mathbf{x}} + \frac{\partial V}{\partial y}\hat{\mathbf{y}} + \frac{\partial V}{\partial z}\hat{\mathbf{z}}, \tag{6.25}$$

which forms a vector-valued function, or a *vector field*. The divergence of a vector field for vector $\mathbf{A}$ is

$$\nabla \cdot \mathbf{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}, \tag{6.26}$$

which is a scalar field. The curl of a vector field is

$$\nabla \times \mathbf{A} = \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right)\hat{\mathbf{x}} + \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right)\hat{\mathbf{y}} + \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\hat{\mathbf{z}}, \tag{6.27}$$

which is still a vector field. The Laplacian operator of a scalar field is

$$\nabla^2 V = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2}, \tag{6.28}$$

which we will study in greater detail in the next chapter.

These operators can be represented in curvilinear coordinates, but we must certainly not write an equation such as

$$\nabla \cdot \mathbf{A} = \frac{\partial A_r}{\partial r} + \frac{\partial A_\theta}{\partial \theta} + \frac{\partial A_\phi}{\partial \phi}, \quad \text{wrongly!}$$

Properties of these differential operators in curvilinear coordinates can be found in any books on electromagnetism; here we simply point out that Maple provides a package `VectorCalculus` that supports all these operators in various coordinate systems. For example, the correct expression of the divergence of a vector field in spherical coordinates is

$$\nabla \cdot \mathbf{A} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 A_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}(\sin\theta A_\theta) + \frac{1}{r\sin\theta}\frac{\partial A_\phi}{\partial \phi}. \tag{6.29}$$

We will discuss these operators in the next chapter.

6.4 Electric Potential

If an electric field is independent of time, the curl of the electric field is always zero:

$$\nabla \times \mathbf{E} = 0. \tag{6.30}$$

This fact allows us to write $\mathbf{E}$ as the gradient of a scalar function V:

$$\mathbf{E} = -\nabla V. \tag{6.31}$$

Gauss's law states that

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}. \tag{6.32}$$

One can show that, for a given charge distribution, V is the integral

$$V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(\mathbf{r}_2)}{r_{12}}\, d\tau_2. \tag{6.33}$$

One advantage of this formula is that, because V is a scalar function, instead of using Coulomb's law directly, which involves three integrals, we only need one. Once V is obtained, the electric field is just its gradient; to differentiate is generally easier than to integrate.

The function V has a physical meaning: it is the electric potential, which is the line integral of the electric field

$$V(\mathbf{r}_1) = \int_{\mathcal{O}}^{\mathbf{r}_1} \mathbf{E} \cdot d\mathbf{l}, \tag{6.34}$$

where $\mathcal{O}$ is a reference point, typically set at infinity. Because the curl of the electric field is zero, the gradient theorem states that the electric potential V is independent of the path of the integral.

If a line charge density λ or a surface charge density σ is given, one writes the integral for the electric potential as

$$V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0}\int \frac{\lambda(\mathbf{r}_2)}{r_{12}}\,dl_2, \quad V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0}\int \frac{\sigma(\mathbf{r}_2)}{r_{12}}\,da_2, \tag{6.33′}$$

respectively.

Example 6.4 Find the electric potential at a distance z above the center of a flat circular disk of radius R that carries a uniform surface charge density; the total charge Q. From the potential, calculate the electric field. Compare the result with that obtained directly from the integral using Coulomb's law.

Solution The surface charge density is

$$\sigma = \frac{Q}{\pi R^2}.$$

The position vector for the field point is

$$\mathbf{r}_1 = z_1\hat{\mathbf{z}}.$$

For this problem, polar coordinates, which are spherical coordinates with $\theta_2 = \pi/2$, are convenient. Adopting the notation of Section 6.2.1, we express the position vector for the source point as

$$\mathbf{r}_2 = r_2\cos\phi_2\hat{\mathbf{x}} + r_2\sin\phi_2\hat{\mathbf{y}},$$

and the length of the separation vector as

$$r_{12} = \sqrt{r_2^2 + z_1^2}.$$

According to equation (6.17), the area element in polar coordinates is

$$da_2 = r_2 dr_2 d\phi_2.$$

Directly from equation (6.33′), we evaluate the electric potential:

$$\begin{aligned} V(\mathbf{r}_1) &= \frac{1}{4\pi\epsilon_0}\int_0^R dr_2\int_0^{2\pi} d\phi_2 \frac{Q}{\pi R^2}\frac{1}{\sqrt{r_2^2+z_1^2}}r_2 \\ &= \frac{Q}{2\pi\epsilon_0 R^2}\left(\sqrt{R^2+z_1^2} - z_1\right). \end{aligned} \tag{6.35}$$

Taking the partial derivative of the electric potential with respect to z, we find the electric field along this direction to be

$$E_z = -\frac{\partial V}{\partial z_1} = \frac{Q}{2\pi\epsilon_0 R^2}\left(1 - \frac{z_1}{\sqrt{z_1^2 + R^2}}\right), \tag{6.36}$$

which agrees with the result obtained from the direct calculation as demonstrated in the worksheet.

Worksheet 6.4 Maintaining our systematic method of defining variables, we readily evaluate the vectors and integrals for the electric potential and field. We verify that the field evaluated from the electric potential, `Ez`, and from direct integration, `Ezp`, are identical.

```
> with(LinearAlgebra):
> assume(z1>0, r2>0, phi2>0, R>0);
> sigma := Q/(Pi*R^2);
```

$$\sigma := \frac{Q}{\pi\, R^2}$$

```
> r2vec := < r2*cos(phi2) | r2*sin(phi2) | 0 >;
```

$$r2vec := [r2\cos(\phi 2),\ r2\sin(\phi 2),\ 0]$$

```
> r1vec := < 0 | 0 | z1 >;
```

$$r1vec := [0,\ 0,\ z1]$$

```
> r12vec := r1vec - r2vec;
```

$$r12vec := [-r2\cos(\phi 2),\ -r2\sin(\phi 2),\ z1]$$

```
> e12 := Normalize(r12vec, 2):
> e12 := map(simplify, e12);
```

$$e12 := \left[-\frac{r2\cos(\phi 2)}{\sqrt{r2^2 + z1^2}},\ -\frac{r2\sin(\phi 2)}{\sqrt{r2^2 + z1^2}},\ \frac{z1}{\sqrt{r2^2 + z1^2}}\right]$$

```
> r12 := Norm(r12vec, 2):
> r12 := simplify(r12);
```

$$r12 := \sqrt{r2^2 + z1^2}$$

```
> Vz := 1/(4*Pi*epsilon[0])*int(int(sigma*r2/r12, phi2=0..2*Pi),
> r2=0..R);
```

$$Vz := -\frac{1}{2}\,\frac{Q\,(-\sqrt{R^2 + z1^2} + z1)}{\pi\,\varepsilon_0\,R^2}$$

```
> Ez := -diff(Vz, z1);
```

$$Ez := \frac{1}{2}\,\frac{Q\,(-\dfrac{z1}{\sqrt{R^2 + z1^2}} + 1)}{\pi\,\varepsilon_0\,R^2}$$

```
> Ezp := 1/(4*Pi*epsilon[0])*int(int(sigma*e12[3]*r2/r12^2,
> phi2=0..2*Pi), r2=0..R);
```

$$Ezp := -\frac{1}{2}\frac{Q\left(-\sqrt{R^2+z1^2}+z1\right)}{\pi\,\varepsilon_0\,\sqrt{R^2+z1^2}\,R^2}$$

Example 6.5 The surface of a right circular cone carries a uniform surface charge density σ. The height of the cone is h, as is the radius of the base. Find the potential difference between points $\mathbf{a}$, the vertex, and $\mathbf{b}$, the center of the top, defined in Figure 6.3.[1]

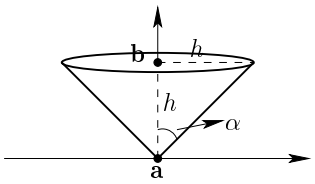


Figure 6.3: A cone carrying a uniform surface charge.

Solution Setting the origin at $\mathbf{a}$, we have

$$\mathbf{r}_{1a} = 0, \quad \mathbf{r}_{1b} = h\hat{\mathbf{z}}.$$

Because the source charge is confined to the cone, we use spherical coordinates at a fixed angle ($\theta = \alpha$); from the configuration,

$$\tan\alpha = 1, \quad \alpha = \frac{\pi}{4}.$$

Therefore,

$$\mathbf{r}_2 = r_2\sin\alpha\cos\phi_2\,\hat{\mathbf{x}} + r_2\sin\alpha\sin\phi_2\,\hat{\mathbf{y}} + r_2\cos\alpha\,\hat{\mathbf{z}},$$

and the separation vectors are

$$\mathbf{r}_{1a2} = \mathbf{r}_{1a} - \mathbf{r}_2, \quad r_{1a2} = r_2$$

$$\mathbf{r}_{1b2} = \mathbf{r}_{1b} - \mathbf{r}_2, \quad r_{1b2} = \sqrt{r_2^2 + h^2 + \sqrt{2}r_2h}.$$

For this problem, the area element on the cone at a fixed θ (at α) is obtained from equation (6.17),

$$da_2 = r_2\sin\alpha\,dr_2\,d\phi_2.$$

[1] Griffiths 1999, p. 87, problem 2.26.

The potential at $\mathbf{a}$ is

$$V_a = \frac{1}{4\pi\epsilon_0}\int_0^{\sqrt{2}h} dr_2 \int_0^{2\pi} d\phi_2 \frac{\sigma}{r_2} r_2 \sin\alpha = \frac{\sigma h}{2\epsilon_0}, \tag{6.37}$$

and at $\mathbf{b}$ is

$$\begin{aligned} V_b &= \frac{1}{4\pi\epsilon_0}\int_0^{\sqrt{2}h} dr_2 \int_0^{2\pi} d\phi_2 \frac{\sigma}{\sqrt{r_2^2 + h^2 + \sqrt{2}r_2 h}} r_2 \sin\alpha \\ &= \frac{\sigma h}{4\epsilon_0}\left[\ln(2+\sqrt{2}) - \ln(2-\sqrt{2})\right]. \end{aligned} \tag{6.38}$$

The potential difference between $\mathbf{a}$ and $\mathbf{b}$ is

$$V_a - V_b = \frac{\sigma h}{2\epsilon_0} - \frac{\sigma h}{4\epsilon_0}\left[\ln(2+\sqrt{2}) - \ln(2-\sqrt{2})\right]. \tag{6.39}$$

Worksheet 6.5 It should be easy to discern the meaning of the symbols because we employ the definitions in a uniform fashion. The calculations are similar to the preceding examples.

```
> with(LinearAlgebra):
> assume(r2>0, phi2, real, h>0);
> alpha := Pi/4;
```

$$\alpha := \frac{\pi}{4}$$

```
> x2:=r2*sin(alpha)*cos(phi2); y2:=r2*sin(alpha)*sin(phi2);
> z2:=r2*cos(alpha);
```

$$x2 := \frac{1}{2}\, r2\, \sqrt{2}\cos(\phi 2)$$

$$y2 := \frac{1}{2}\, r2\, \sqrt{2}\sin(\phi 2)$$

$$z2 := \frac{r2\,\sqrt{2}}{2}$$

```
> r2vec := < x2 | y2 | z2 >;
```

$$r2vec := \left[\frac{1}{2}\, r2\, \sqrt{2}\cos(\phi 2),\ \frac{1}{2}\, r2\, \sqrt{2}\sin(\phi 2),\ \frac{r2\,\sqrt{2}}{2}\right]$$

```
> r1a := < 0 | 0 | 0 >;
```

$$r1a := [0,\ 0,\ 0]$$

```
> r1b := < 0 | 0 | h >;
```

$$r1b := [0,\ 0,\ h]$$

```
> r1a2vec := r1a - r2vec;
```

$$r1a2vec := \left[-\frac{1}{2}\,r2\,\sqrt{2}\cos(\phi 2),\ -\frac{1}{2}\,r2\,\sqrt{2}\sin(\phi 2),\ -\frac{r2\,\sqrt{2}}{2}\right]$$

```
> r1b2vec := r1b - r2vec;
```

$$r1b2vec := \left[-\frac{1}{2}\,r2\,\sqrt{2}\cos(\phi 2),\ -\frac{1}{2}\,r2\,\sqrt{2}\sin(\phi 2),\ h-\frac{r2\,\sqrt{2}}{2}\right]$$

```
> r1a2 := Norm(r1a2vec, 2):
> r1b2 := Norm(r1b2vec, 2):
> r1a2 := simplify(r1a2);
```

$$r1a2 := r2$$

```
> r1b2 := simplify(r1b2);
```

$$r1b2 := \sqrt{r2^2+h^2-h\,r2\,\sqrt{2}}$$

```
> Va := 1/(4*Pi*epsilon[0])* int(int(sigma*r2*sin(alpha)/r1a2,
> phi2=0..2*Pi), r2=0..h/sin(alpha));
```

$$Va := \frac{1}{2}\,\frac{\sigma\,h}{\varepsilon_0}$$

```
> Vb := 1/(4*Pi*epsilon[0])* int(int(sigma*r2*sin(alpha)/r1b2,
> phi2=0..2*Pi), r2=0..h/sin(alpha));
```

$$Vb := \frac{1}{4}\,\frac{\sigma\,\pi\,h\ln(2+\sqrt{2})-\sigma\,\pi\,h\ln(2-\sqrt{2})}{\pi\,\varepsilon_0}$$

```
> simplify(Va - Vb);
```

$$\frac{1}{4}\,\frac{\sigma\,h\,(2-\ln(2+\sqrt{2})+\ln(2-\sqrt{2}))}{\varepsilon_0}$$

6.4.1 Cavendish's Apparatus for the Inverse Square Law

Gauss's law in equation (6.32) is true only because the Coulomb force depends exactly on the inverse square of the distance. Before Coulomb published his force law, Benjamin Franklin noticed that the field inside a conducting shell is zero, and he reported his observation to Joseph Priestley. Because a spherical shell of matter produced no gravitational field inside, Priestley suggested that electric force, like gravitational force, also has an inverse square dependence on distance. Henry Cavendish later devised an experiment to investigate this phenomenon.[2] Cavendish's apparatus consists of two concentric spherical conducting shells; the inner shell was first charged, then connected to the outer shell. On testing the inner shell for

[2]For a facsimile of Cavendish's own sketch, see Jackson 1999, p. 6.

charge, it was found that the inner shell possessed no charge (to the precision of his electroscope). Cavendish thus discovered the inverse square nature of the electric force in 1776, before Coulomb showed that the force between electric charges had the same form as the gravitational force, in 1785.

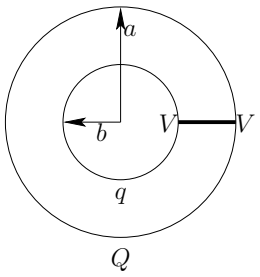


Figure 6.4: Cavendish's apparatus for the inverse square law.

Cavendish's apparatus serves to test the validity of the inverse square law; see Figure 6.4. Suppose that the exponent in the force law differs from 2 by δ,

$$\mathbf{F} = \frac{1}{4\pi\epsilon_0}\frac{q_1 q_2}{r_{12}^{2-\delta}}\mathbf{e}_{12}, \tag{6.40}$$

then the charge on the inner shell would not be exactly zero, and the amount of charge depends on δ. The potential due to a point charge q_2 under this proposed force law would be

$$V(\mathbf{r}_1) = \int_{\infty}^{\mathbf{r}_1} \mathbf{E}\cdot d\mathbf{l} = \frac{1}{4\pi\epsilon_0}\int_{\infty}^{r1}\frac{q_2}{r^{2-\delta}}dr = \frac{1}{4\pi\epsilon_0(1-\delta)}\frac{q_2}{r^{1-\delta}}.$$

For a continuous charge distribution, we modify equation (6.33′) accordingly:

$$V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0(1-\delta)}\int\frac{\sigma(\mathbf{r}_2)}{r_{12}^{1-\delta}}da_2. \tag{6.41}$$

With this proposed force law, we calculate the potential produced by a spherical shell of radius R with a uniform charge density

$$\sigma(\mathbf{r}_2) = \frac{\Xi}{4\pi R^2},$$

where Ξ is the total charge. Because of spherical symmetry, we align the position vector of the field point with the z axis,

$$\mathbf{r}_1 = z_1\hat{\mathbf{z}};$$

the position vector of the source point on the shell of radius R is

$$\mathbf{r}_2 = |\mathbf{r}_1 - \mathbf{r}_2| = R\sin\theta_2\cos\phi_2\,\hat{\mathbf{x}} + R\sin\theta_2\sin\phi_2\,\hat{\mathbf{y}} + R\cos\theta_2\,\hat{\mathbf{z}},$$

and the area element for the shell is

$$da_2 = R^2 \sin\theta_2 d\theta_2 d\phi_2.$$

The length of the separation vector follows directly:

$$r_{12} = \sqrt{R^2 + z_1^2 - 2Rz_1\cos\theta_2}.$$

The integral for potential is elementary, but the result depends on whether z_1 is inside or outside the shell:

$$V_{\text{out}}(z_1, \Xi, R) = \frac{1}{4\pi\epsilon_0}\frac{\Xi}{2(1-\delta^2)Rz_1}\Big\{R\left[(z_1+R)^\delta + (z_1-R)^\delta\right] + z_1\left[(z_1+R)^\delta - (z_1-R)^\delta\right]\Big\}, \quad (6.42a)$$

$$V_{\text{in}}(z_1, \Xi, R) = \frac{1}{4\pi\epsilon_0}\frac{\Xi}{2(1-\delta^2)Rz_1}\Big\{R\left[(R+z_1)^\delta - (R-z_1)^\delta\right] + z_1\left[(R+z_1)^\delta + (R-z_1)^\delta\right]\Big\}. \quad (6.42b)$$

One should notice that when $\delta = 0$, the potential inside the shell is constant, thus there is no field, and the potential outside the shell is identical to that due to a point charge.

Suppose that Cavendish's experiment resulted in q on the inner shell and Q on the outer shell (Figure 6.4). The potential V_a of the outer shell ($z_1 = a$) is contributed from charge on the outer shell Q, and charge on the inner shell q, and we use V_{out} for both:

$$V_a = V_{\text{out}}(z_1 = a, \Xi = Q, R = a) + V_{\text{out}}(z_1 = a, \Xi = q, R = b). \quad (6.43a)$$

The potential of the inner shell ($z_1 = b$) is also contributed from charge on the outer shell Q, and charge on the inner shell q, but we use V_{in} for the former:

$$V_b = V_{\text{in}}(z_1 = b, \Xi = Q, R = a) + V_{\text{out}}(z_1 = b, \Xi = q, R = b). \quad (6.43b)$$

Because the shells are connected, the potential must be the same, say V_0, we have

$$V_a = V_0, \quad V_b = V_0.$$

Solving these two equations simultaneously, we obtain q and Q; see the Maple worksheet below for somewhat long expressions. For small δ, we expand q and obtain

$$q = \frac{2\pi\epsilon_0 V_0 a\delta}{a-b}\left[b\ln\left(\frac{4a^2}{a^2-b^2}\right) - b\ln\left(\frac{a+b}{a-b}\right)\right]. \quad (6.44)$$

Measuring q thus allows the determination of δ.

Worksheet 6.6 The calculations are similar to previous examples, except for a modification of the exponent of r_{12}.

```
> with(LinearAlgebra):
> sigma := Xi/(4*Pi*R^2);
```

$$\sigma := \frac{\Xi}{4\,\pi\,R^2}$$

```
> r2vec := < R*sin(theta2)*cos(phi2) | R*sin(theta2)*sin(phi2) |
> R*cos(theta2) >;
```

$$r2vec := [R\sin(\theta 2)\cos(\phi 2),\ R\sin(\theta 2)\sin(\phi 2),\ R\cos(\theta 2)]$$

```
> r1vec := < 0 | 0 | z1 >;
```

$$r1vec := [0,\ 0,\ z1]$$

```
> r12vec := r1vec - r2vec:
> r12 := Norm(r12vec, 2):
> r12 := simplify(r12) assuming R>0, z1>0, theta2>0, phi2>0;
```

$$r12 := \sqrt{R^2 + z1^2 - 2\,z1\,R\cos(\theta 2)}$$

```
> V := 1/(4*Pi*epsilon[0]*(1-delta))
> *int(int(sigma*R^2*sin(theta2)/r12^(1-delta), phi2=0..2*Pi),
> theta2=0..Pi);
```

$$V := \frac{1}{4}\left(\frac{1}{\pi\,\varepsilon_0\,(1-\delta)}\int_0^{\pi}\frac{1}{2}\,\frac{\Xi\sin(\theta 2)}{(\sqrt{R^2 + z1^2 - 2\,z1\,R\cos(\theta 2)})^{(1-\delta)}}\,d\theta 2\right)$$

```
> Vout := simplify(V) assuming R>0, z1>0, z1>R;
```

$$Vout := -\frac{1}{8}\Xi(\sqrt{(R^2 + z1^2 + 2\,z1\,R)^{\delta}}\,R + \sqrt{(R^2 + z1^2 + 2\,z1\,R)^{\delta}}\,z1$$
$$-\sqrt{(R^2 + z1^2 - 2\,z1\,R)^{\delta}}\,z1 + \sqrt{(R^2 + z1^2 - 2\,z1\,R)^{\delta}}\,R)\Big/(\pi\,\varepsilon_0\,z1\,R\,(-1+\delta^2))$$

```
> Vin := simplify(V) assuming R>0, z1>0, z1<R;
```

$$Vin := -\frac{1}{8}\Xi(\sqrt{(R^2 + z1^2 + 2\,z1\,R)^{\delta}}\,R + \sqrt{(R^2 + z1^2 + 2\,z1\,R)^{\delta}}\,z1$$
$$-\sqrt{(R^2 + z1^2 - 2\,z1\,R)^{\delta}}\,R + \sqrt{(R^2 + z1^2 - 2\,z1\,R)^{\delta}}\,z1)\Big/(\pi\,\varepsilon_0\,z1\,R\,(-1+\delta^2))$$

```
> assume(a>b):
> Va := eval(Vout, {z1=a, Xi=Q, R=a}) + eval(Vout, {z1=a, Xi=q,
> R=b});
```

$$Va := -\frac{1}{4}\,\frac{Q\,\sqrt{(4\,a^2)^{\delta}}}{\pi\,\varepsilon_0\,a\,(-1+\delta^2)} - \frac{1}{8}q(\sqrt{(b^2 + a^2 + 2\,a\,b)^{\delta}}\,b + \sqrt{(b^2 + a^2 + 2\,a\,b)^{\delta}}\,a$$
$$-\sqrt{(b^2 + a^2 - 2\,a\,b)^{\delta}}\,a + \sqrt{(b^2 + a^2 - 2\,a\,b)^{\delta}}\,b)\Big/(\pi\,\varepsilon_0\,a\,b\,(-1+\delta^2))$$

```
> Vb := eval(Vin, {z1=b, Xi=Q, R=a}) + eval(Vout, {z1=b, Xi=q,
> R=b});
```

$$Vb := -\frac{1}{8}Q(\sqrt{(b^2+a^2+2\,a\,b)^{\delta}}\,b+\sqrt{(b^2+a^2+2\,a\,b)^{\delta}}\,a-\sqrt{(b^2+a^2-2\,a\,b)^{\delta}}\,a$$
$$+\sqrt{(b^2+a^2-2\,a\,b)^{\delta}}\,b)\Big/(\pi\,\varepsilon_0\,b\,a\,(-1+\delta^2))-\frac{1}{4}\,\frac{q\,\sqrt{(4\,b^2)^{\delta}}}{\pi\,\varepsilon_0\,b\,(-1+\delta^2)}$$

```
> Eq1 := Va = V0;
```

$$Eq1 := -\frac{1}{4}\,\frac{Q\,\sqrt{(4\,a^2)^{\delta}}}{\pi\,\varepsilon_0\,a\,(-1+\delta^2)}-\frac{1}{8}q(\sqrt{(b^2+a^2+2\,a\,b)^{\delta}}\,b+\sqrt{(b^2+a^2+2\,a\,b)^{\delta}}\,a$$
$$-\sqrt{(b^2+a^2-2\,a\,b)^{\delta}}\,a+\sqrt{(b^2+a^2-2\,a\,b)^{\delta}}\,b)\Big/(\pi\,\varepsilon_0\,a\,b\,(-1+\delta^2))=V0$$

```
> Eq2 := Vb = V0;
```

$$Eq2 := -\frac{1}{8}Q(\sqrt{(b^2+a^2+2\,a\,b)^{\delta}}\,b+\sqrt{(b^2+a^2+2\,a\,b)^{\delta}}\,a-\sqrt{(b^2+a^2-2\,a\,b)^{\delta}}\,a$$
$$+\sqrt{(b^2+a^2-2\,a\,b)^{\delta}}\,b)\Big/(\pi\,\varepsilon_0\,b\,a\,(-1+\delta^2))-\frac{1}{4}\,\frac{q\,\sqrt{(4\,b^2)^{\delta}}}{\pi\,\varepsilon_0\,b\,(-1+\delta^2)}=V0$$

```
> Soln1 := solve({Eq1, Eq2}, {Q, q}):
> assign(Soln1);
> q;
```

$$-8\,V0\,\pi\,\varepsilon_0\,a\,b(\sqrt{\%1}\,b-\sqrt{\%1}\,b\,\delta^2+\sqrt{\%2}\,b-\sqrt{\%2}\,b\,\delta^2+\sqrt{\%2}\,a-\sqrt{\%2}\,a\,\delta^2$$
$$-\sqrt{\%1}\,a+\sqrt{\%1}\,a\,\delta^2-2\,\sqrt{(4\,a^2)^{\delta}}\,b+2\,b\,\delta^2\,\sqrt{(4\,a^2)^{\delta}})\Big/(-2\,\sqrt{\%1}\,b^2\,\sqrt{\%2}$$
$$+2\,\%1\,b\,a-\%1\,b^2-\%2\,b^2-2\,\%2\,b\,a-\%2\,a^2+2\,\sqrt{\%2}\,a^2\,\sqrt{\%1}-\%1\,a^2$$
$$+4\,\sqrt{(4\,b^2)^{\delta}}\,a\,\sqrt{(4\,a^2)^{\delta}}\,b)$$
$$\%1 := (b^2+a^2-2\,a\,b)^{\delta}$$
$$\%2 := (b^2+a^2+2\,a\,b)^{\delta}$$

```
> simplify(taylor(q, delta, 2));
```

$$V0\,\pi\,\varepsilon_0\,a(-2\ln(a-b)\,b-\ln((a+b)^2)\,b-\ln((a+b)^2)\,a+2\ln(a-b)\,a+4\,b\ln(2)$$
$$+2\,b\ln(a^2))/(a-b)\delta+\mathrm{O}(\delta^2)$$

6.4.2 Multipole Expansion

In calculating the electric field and the potential, the integrals invariably involve the length of the separation vector r_{12}. In previous examples with spherical coordinates, we have restricted ourselves to a special situation where the position vector of the field point $\mathbf{r}_1$ lies on the z axis,

so that

$$r_{12} = \sqrt{z_1^2 + r_2^2 - 2z_1 r_2 \cos\theta_2},$$

and we have successfully evaluated the field and potential under this configuration. We do not always have the symmetry, and it is usually impossible to evaluate the integral exactly. For the most general $\mathbf{r}_1$ and $\mathbf{r}_2$ in spherical coordinates (see Figure 6.5), we have

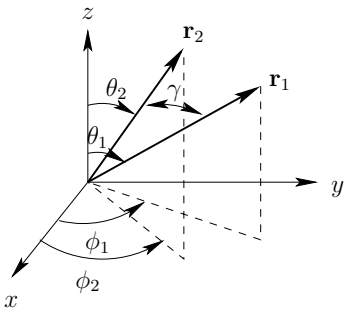


Figure 6.5: Two vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ with spherical coordinates.

$$\mathbf{r}_1 = r_1 \sin\theta_1 \cos\phi_1 \,\hat{\mathbf{x}} + r_1 \sin\theta_1 \sin\phi_1 \,\hat{\mathbf{y}} + r_1 \cos\theta_1 \,\hat{\mathbf{z}},$$

$$\mathbf{r}_2 = r_2 \sin\theta_2 \cos\phi_2 \,\hat{\mathbf{x}} + r_2 \sin\theta_2 \sin\phi_2 \,\hat{\mathbf{y}} + r_2 \cos\theta_2 \,\hat{\mathbf{z}},$$

thus

$$r_{12} = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\gamma}, \tag{6.45a}$$

where γ is the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$, and

$$\cos\gamma = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2). \tag{6.45b}$$

For $r_1 > r_2$, we can write

$$\frac{1}{r_{12}} = \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\gamma}} = \frac{1}{r_1 \sqrt{1 + \left(\frac{r_2}{r_1}\right)^2 - 2\left(\frac{r_2}{r_1}\right)\cos\gamma}}$$

and expand $1/r_{12}$ as a power series of r_2/r_1:

$$\frac{1}{r_{12}} = |\mathbf{r}_1 - \mathbf{r}_2| = \frac{1}{r_1} \sum_l C_l(\cos\gamma) \left(\frac{r_2}{r_1}\right)^l;$$

such a task is suitable for Maple.

Worksheet 6.7 We use the `taylor` command to perform the series expansion. We remind the reader that `gamma` is pre-defined as Euler's constant in Maple; although we use it to display the symbol γ, one should avoid using it in an actual calculation.

```
> r12 := 1/sqrt(r1^2 + r2^2 - 2*r1*r2*cos(gamma));
```

$$r12 := \frac{1}{\sqrt{r1^2 + r2^2 - 2\,r1\,r2\cos(\gamma)}}$$

```
> taylor(r12, r2) assuming r1>0;
```

$$\frac{1}{r1} + \frac{\cos(\gamma)}{r1^2}\,r2 + \frac{-\frac{1}{2\,r1^2} + \frac{3}{2}\frac{\cos(\gamma)^2}{r1^2}}{r1}\,r2^2 + \frac{-\frac{3}{2}\frac{\cos(\gamma)}{r1^3} + \frac{5}{2}\frac{\cos(\gamma)^3}{r1^3}}{r1}\,r2^3 + \frac{\frac{3}{8\,r1^4} - \frac{15}{4}\frac{\cos(\gamma)^2}{r1^4} + \frac{35}{8}\frac{\cos(\gamma)^4}{r1^4}}{r1}\,r2^4 + \frac{\frac{15}{8}\frac{\cos(\gamma)}{r1^5} - \frac{35}{4}\frac{\cos(\gamma)^3}{r1^5} + \frac{63}{8}\frac{\cos(\gamma)^5}{r1^5}}{r1}\,r2^5 + \mathrm{O}(r2^6)$$

The expansion shows that C_l is none other than the Legendre polynomials P_l introduced in the preceding chapter (see Table 5.1). Such a result should not be a surprise because $|\mathbf{r}_1 - \mathbf{r}_2|^{-1}$ is simply the generating function of Legendre polynomials; in other words, the length of the separation vector provides a simple geometrical interpretation of the generating function for the Legendre polynomials introduced in Section 5.4.1. We list the first five Legendre polynomials again:

$$\begin{aligned}
P_0(\cos\gamma) &= 1,\\
P_1(\cos\gamma) &= \cos\gamma,\\
P_2(\cos\gamma) &= \frac{3}{2}\cos^2\gamma - \frac{1}{2},\\
P_3(\cos\gamma) &= \frac{5}{2}\cos^3\gamma - \frac{3}{2}\cos\gamma,\\
P_4(\cos\gamma) &= \frac{35}{8}\cos^4\gamma - \frac{15}{4}\cos^2\gamma + \frac{3}{8},\\
P_5(\cos\gamma) &= \frac{63}{8}\cos^5\gamma - \frac{35}{4}\cos^3\gamma + \frac{15}{8}\cos\gamma.
\end{aligned}$$

With these Legendre polynomials, $1/r_{12}$ becomes

$$\frac{1}{r_{12}} = \sum_{l=0}^{\infty} \frac{r_2^l}{r_1^{l+1}} P_l(\cos\gamma), \quad \text{for } r_1 > r_2. \tag{6.46}$$

For $r_1 < r_2$, we need only to interchange r_1 and r_2. In a compact notation, we write

$$\frac{1}{r_{12}} = \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\gamma), \tag{6.47}$$

where $r_<$ ($r_>$) is the smaller (larger) of $|\mathbf{r}_1|$ and $|\mathbf{r}_2|$.

The addition theorem of spherical harmonics allows a further expansion of $P(\cos\gamma)$.[3] We will wait until our treatment of quantum mechanics to discuss spherical harmonics (see equation (16.20)). Here we consider a situation when the charge distribution does not depend on ϕ, namely a configuration with azimuthal symmetry. We leave it for the reader to perform the integral to verify that

$$\langle P_l(\cos\gamma)\rangle_{\text{averaged over }\phi_2} = \frac{1}{2\pi}\int_0^{2\pi} P_l(\cos\gamma)d\phi_2 = P_l(\cos\theta_1)P_l(\cos\theta_2). \tag{6.48}$$

Therefore, if the charge distribution of the source has azimuthal symmetry, the expansion of r_{12} is[4]

$$\left\langle \frac{1}{r_{12}} \right\rangle_{\text{averaged over }\phi_2} = \sum_{l=0}^{\infty} \frac{r_2^l}{r_1^{l+1}} P_l(\cos\theta_1)P_l(\cos\theta_2), \quad \text{for } r_1 > r_2. \tag{6.49}$$

With $1/r_{12}$ expressed as a sum of the Legendre polynomials, it is convenient to express the potential as a multipole expansion. Using the integral in equation (6.33), we write

$$V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0}\sum_{l=0}^{\infty} q_l \frac{P_l(\cos\theta_1)}{r_1^{l+1}} \tag{6.50}$$

where

$$q_l = \int r_2^l P_l(\cos\theta_2)\rho(\mathbf{r}_2)d\tau_2. \tag{6.51}$$

these q_l terms are the 2^l-pole moments. For example,

$$q_0 = \int \rho(\mathbf{r}_2)d\tau_2$$

signifies the total charge or the monopole moment,

$$q_1 = \int r_2\cos\theta_2\rho(\mathbf{r}_2)d\tau_2$$

is the dipole moment, and

$$q_2 = \int r_2^2\left(\frac{3}{2}\cos^2\theta_2 - \frac{1}{2}\right)\rho(\mathbf{r}_2)d\tau_2$$

is the quadrupole moment. The potential contributed by each 2^n-pole moment decreases as $1/r^{l+1}$.

Example 6.6 In an earlier example we found the electric potential on the z axis above a flat circular disk of radius R that carries a total charge Q uniformly distributed over the disk. Now we want to find the electric potential anywhere above the disk; see Figure 6.6.

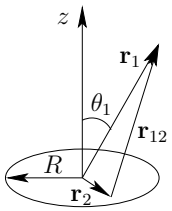


Figure 6.6: Potential above a charged disk.

Solution To find the potential far from the source, we employ the technique of multipole expansion. The disk has a charge density

$$\sigma(\mathbf{r}_2) = \frac{Q}{\pi R^2}.$$

Because the disk is on the xy plane, $\theta_2 = \pi/2$; the area element for the disk is

$$da_2 = 2\pi r_2 dr_2.$$

The calculation of multipole moments is straightforward. We have

$$\begin{aligned}
q_0 &= 2\pi \int_0^R dr_2 P_0\left(\cos\frac{\pi}{2}\right)\sigma(\mathbf{r}_2) r_2 = Q,\\
q_2 &= 2\pi \int_0^R dr_2 r_2^2 P_2\left(\cos\frac{\pi}{2}\right)\sigma(\mathbf{r}_2) r_2 = -\frac{QR^2}{4},\\
q_4 &= 2\pi \int_0^R dr_2 r_2^4 P_4\left(\cos\frac{\pi}{2}\right)\sigma(\mathbf{r}_2) r_2 = \frac{QR^4}{8},\\
&\ldots,\\
q_l &= 2\pi \int_0^R dr_2 r_2^l P_l\left(\cos\frac{\pi}{2}\right)\sigma(\mathbf{r}_2) r_2.
\end{aligned}$$

Recall that $P_l(0) = 0$ for odd l. The potential as a multipole expansion is

$$V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0}\frac{Q}{r_1}\left[1 - \frac{1}{4}\left(\frac{R}{r}\right)^2 P_2(\cos\theta_1) + \frac{1}{8}\left(\frac{R}{r}\right)^4 P_4(\cos\theta_1) - \frac{5}{64}\left(\frac{R}{r}\right)^6 P_6(\cos\theta_1) + \ldots\right], \quad (6.52)$$

where

$$P_0(\cos\theta_1) = 1,$$

[3] Jackson 1999, equation (3.62) p. 110.

[4] In Griffiths 1999, equation (3.94), p. 148, $\mathbf{r}_1$ is aligned with the z axis (which makes $\theta_1 \equiv 0$), so $P_l(\cos\theta_1) = 1$ does not appear in his expansion of $1/r_{12}$.

$$P_2(\cos\theta_1) = \frac{3}{2}\cos^2\theta_1 - \frac{1}{2},$$

$$P_4(\cos\theta_1) = \frac{35}{8}\cos^4\theta_1 - \frac{15}{4}\cos^2\theta_1 + \frac{3}{8},$$

$$P_6(\cos\theta_1) = \frac{231}{16}\cos^6\theta_1 - \frac{315}{16}\cos^4\theta_1 + \frac{105}{16}\cos^2\theta_1 - \frac{5}{16}.$$

Worksheet 6.8 Recall that the Legendre polynomials is defined as `LegendreP`; Maple can perform these elementary integrals.

```
> sigma := Q/(Pi*R^2);
```

$$\sigma := \frac{Q}{\pi R^2}$$

```
> theta2 := Pi/2;
```

$$\theta 2 := \frac{\pi}{2}$$

```
> q0 := int(r2^0*LegendreP(0, cos(theta2))*sigma*2*Pi*r2, r2=0..R);
```

$$q0 := Q$$

```
> q1 := int(r2^1*LegendreP(1, cos(theta2))*sigma*2*Pi*r2, r2=0..R);
```

$$q1 := 0$$

```
> q2 := int(r2^2*LegendreP(2, cos(theta2))*sigma*2*Pi*r2, r2=0..R);
```

$$q2 := -\frac{Q\,R^2}{4}$$

```
> q3 := int(r2^3*LegendreP(3, cos(theta2))*sigma*2*Pi*r2, r2=0..R);
```

$$q3 := 0$$

```
> q4 := int(r2^4*LegendreP(4, cos(theta2))*sigma*2*Pi*r2, r2=0..R);
```

$$q4 := \frac{Q\,R^4}{8}$$

```
> q5 := int(r2^5*LegendreP(5, cos(theta2))*sigma*2*Pi*r2, r2=0..R);
```

$$q5 := 0$$

```
> q6 := int(r2^6*LegendreP(6, cos(theta2))*sigma*2*Pi*r2, r2=0..R);
```

$$q6 := -\frac{5\,Q\,R^6}{64}$$

```
> V := 1/(4*Pi*epsilon[0])*(q0*LegendreP(0, cos(theta1))/(r1) +
q2*expand(LegendreP(2, cos(theta1)))/r1^3 + q4*expand(LegendreP(4,
cos(theta1)))/r1^5 + q6*expand(LegendreP(6, cos(theta1)))/r1^7);
```

$$V := \frac{1}{4}\left(\frac{Q}{r1} - \frac{1}{4}\frac{Q\,R^2\left(-\frac{1}{2}+\frac{3}{2}\cos(\theta1)^2\right)}{r1^3} + \frac{1}{8}\frac{Q\,R^4\left(\frac{3}{8}+\frac{35}{8}\cos(\theta1)^4-\frac{15}{4}\cos(\theta1)^2\right)}{r1^5}\right.$$
$$\left. - \frac{5}{64}\,\frac{Q\,R^6\left(-\frac{5}{16}+\frac{231}{16}\cos(\theta1)^6-\frac{315}{16}\cos(\theta1)^4+\frac{105}{16}\cos(\theta1)^2\right)}{r1^7}\right)\Big/(\pi\,\varepsilon_0)$$

Example 6.7 A sphere of radius R, centered at the origin, carries charge density

$$\rho(r_2,\theta_2) = k\frac{R}{r_2}(R-2r_2)\sin\theta_2,$$

where k is a constant, and r_2 and θ_2 are the usual spherical coordinates. Find the potential outside the sphere. This is problem 3.26 in Griffiths 1999, p. 149, but we do not restrict ourselves on the z axis.

Solution The volume element in spherical coordinates is

$$d\tau_2 = 2\pi r_2^2 \sin\theta_2 dr_2 d\theta_2,$$

and the calculation is straightforward. We only list three nonvanishing multipole moments:

$$q_2 = 2\pi\int_0^R dr_2 r_2^2 P_2(\cos\theta_2)\,\rho(\mathbf{r}_2) r_2^2\sin\theta_2 = \frac{k\pi^2R^5}{48},$$

$$q_4 = 2\pi\int_0^R dr_2 r_2^4 P_4(\cos\theta_2)\,\rho(\mathbf{r}_2) r_2^2\sin\theta_2 = \frac{k\pi^2R^7}{480},$$

$$q_6 = 2\pi\int_0^R dr_2 r_2^6 P_6(\cos\theta_2)\,\rho(\mathbf{r}_2) r_2^2\sin\theta_2 = \frac{15k\pi^2R^9}{28672}.$$

The potential as a multipole expansion is

$$V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0}\left[\frac{k\pi^2R^5}{48r_1^3}P_2(\cos\theta_1) + \frac{k\pi^2R^7}{480r_1^5}P_4(\cos\theta_1)\right.$$
$$\left. + \frac{15k\pi^2R^9}{28672r_1^7}P_6(\cos\theta_1) + \ldots\right]. \quad (6.53)$$

Worksheet 6.9 The calculation is completely analogous to the preceding example.

```
> rho := k*R/r2^2*(R-2*r2)*sin(theta2);
```

$$\rho := \frac{k\,R\,(R-2\,r2)\sin(\theta 2)}{r2^2}$$

```
> q2 := int(int(r2^2*LegendreP(2,
> cos(theta2))*rho*2*Pi*r2^2*sin(theta2), theta2=0..Pi), r2=0..R);
```

$$q2 := \frac{\pi^2\,k\,R^5}{48}$$

```
> q4 := int(int(r2^4*LegendreP(4,
> cos(theta2))*rho*2*Pi*r2^2*sin(theta2), theta2=0..Pi), r2=0..R);
```

$$q4 := \frac{\pi^2\,k\,R^7}{480}$$

```
> q6 := int(int(r2^6*LegendreP(6,
> cos(theta2))*rho*2*Pi*r2^2*sin(theta2), theta2=0..Pi), r2=0..R);
```

$$q6 := \frac{15\,\pi^2\,k\,R^9}{28672}$$

```
> V:=1/(4*Pi*epsilon[0])*(q2*expand(LegendreP(2,cos(theta1)))/r1^3
> + q4*expand(LegendreP(4, cos(theta1)))/r1^5 +
q6*expand(LegendreP(6,
> cos(theta1)))/r1^7);
```

$$V := \frac{1}{4}\left(\frac{1}{48}\frac{\pi^2 k\,R^5\left(-\frac{1}{2}+\frac{3}{2}\cos(\theta 1)^2\right)}{r1^3}+\frac{1}{480}\frac{\pi^2 k\,R^7\left(\frac{3}{8}+\frac{35}{8}\cos(\theta 1)^4-\frac{15}{4}\cos(\theta 1)^2\right)}{r1^5}\right.$$
$$\left.+\frac{15}{28672}\,\frac{\pi^2\,k\,R^9\left(-\frac{5}{16}+\frac{231}{16}\cos(\theta 1)^6-\frac{315}{16}\cos(\theta 1)^4+\frac{105}{16}\cos(\theta 1)^2\right)}{r1^7}\right)\Big/(\pi\,\varepsilon_0)$$

6.5 Electric Field and Equipotential

In this chapter our objective is to calculate the electric field, which is considered to be a fundamental quantity. From an operational point of view, once we determine the electric field, we can obtain force, energy, momentum and angular momentum in space, which convey physical information.

An approach to determine the electric field is through finding the electric potential; we will devote the entire next chapter to this subject. Knowing the electric potential, its gradient gives the electric field. A surface over which the potential is constant is called an equipotential surface; an intersection of an equipotential surface and a plane produces a line known as an equipotential line. The direction of an electric field vector is normal to an equipotential surface.

Because the concept of field might seem abstract, we use the graphic capacity of Maple to offer a pictorial description. Recall that a *field* is a function that specifies a particular quantity at every point of a region; it may or may not depend on time. A scalar field u has a value $u(x, y, z)$ at position (x, y, z) in a three-dimensional space. A vector field $\mathbf{v}$ comprises three functions: at a position (x, y, z), it returns three values: $v_x(x, y, z)$, $v_y(x, y, z)$ and $v_z(x, y, z)$, which are components of a vector. The electric potential satisfies properties of a scalar field, and the electric field satisfies properties of a vector field. That is, at a given point (x, y, z), we have $V(x, y, z)$ and

$$\mathbf{E}(x, y, z) = E_x(x, y, z)\hat{\mathbf{x}} + E_y(x, y, z)\hat{\mathbf{y}} + E_z(x, y, z)\hat{\mathbf{z}}.$$

To graphically present a scalar field, we can only imagine that we plot an explicit function of three variables; alternatively, we can make an implicit plot in three dimensions for the equation

$$V(x, y, z) = \text{constant},$$

which is none other than an equipotential surface. To graphically present a vector field, at any point (x, y, z) we can draw an arrow through the point with components (E_x, E_y, E_z); a collection of these arrows shows the direction of the field. Maple directly generates such a plot of a vector field with the `fieldplot3d` command in the `plots` package. Because it is impossible to plot an explicit function of three variables, and as it is difficult to visualize a three-dimensional implicit plot or vector field, we generally hold a third coordinate constant so that we suppress one dimension from contention. For instance, if we fix z at 0, we can plot both $V(x, y, 0)$ and the projection of the vector field on the xy plane, $[E_x(x, y, 0), E_y(x, y, 0)]$.

Here we illustrate an equipotential surface and its relation to an electric field.

Example 6.8 An electric dipole consists of two charges of equal magnitude but opposite sign a distance apart. Consider a situation in which a positive charge is placed at, neglecting units, $(1, 0, 0)$, and a negative charge is placed at $(-1, 0, 0)$, using the Cartesian basis. Calculate the electric potential and electric field that this dipole produces.

Solution Because we have discrete point charges, instead of integration we form a sum of two terms, neglecting a factor of $1/4\pi\epsilon_0$:

$$V = \frac{1}{\sqrt{(x-1)^2 + y^2 + z^2}} + \frac{-1}{\sqrt{(x+1)^2 + y^2 + z^2}}. \tag{6.54}$$

In this expression for the field point we discard the customary subscript, so we write x instead of x_1, and so forth. From the potential, we evaluate the electric field:

$$\mathbf{E} = -\nabla V = \left\{ \frac{x-1}{[(x-1)^2+y^2+z^2]^{3/2}} - \frac{x+1}{[(x+1)^2+y^2+z^2]^{3/2}} \right\} \hat{\mathbf{x}} + \left\{ \frac{y}{[(x-1)^2+y^2+z^2]^{3/2}} - \frac{y}{[(x+1)^2+y^2+z^2]^{3/2}} \right\} \hat{\mathbf{y}} + \left\{ \frac{z}{[(x-1)^2+y^2+z^2]^{3/2}} - \frac{z}{[(x+1)^2+y^2+z^2]^{3/2}} \right\} \hat{\mathbf{z}}. \quad (6.55)$$

We visualize surfaces of equipotential by projecting them onto a plane, so as to generate contours of equipotential lines. If we choose such a plane to be xy, the contours are implicit plots of the equation

$$V(x, y, 0) = \text{constant}.$$

Worksheet 6.10 For a given potential $V(x, y, z)$, we find its gradient with the `Gradient` command in the `VectorCalculus` package. Maple returns the gradient of V as a vector field, expressed with both components and basis vectors. We employ the `fieldplot3d` command in the `plots` package to present the vector field. By normalizing each vector in this field to unit length using the `Normalize` command, we improve the appearance of the plot to show the directions of the vectors. We apply the `implicitplot` command to generate the equipotential lines.

```
> V := 1/sqrt((x-1)^2 + y^2 + z^2) - 1/sqrt((x+1)^2 + y^2 + z^2);
```

$$V := \frac{1}{\sqrt{x^2-2x+1+y^2+z^2}} - \frac{1}{\sqrt{x^2+2x+1+y^2+z^2}}$$

```
> with(LinearAlgebra): with(VectorCalculus): with(plots):

> with(plottools):

Warning, the names CrossProduct and DotProduct have been rebound

Warning, the assigned names <,> and <|> now have a global binding

Warning, these protected names have been redefined and unprotected: *,
+, ., Vector, diff, int, limit, series

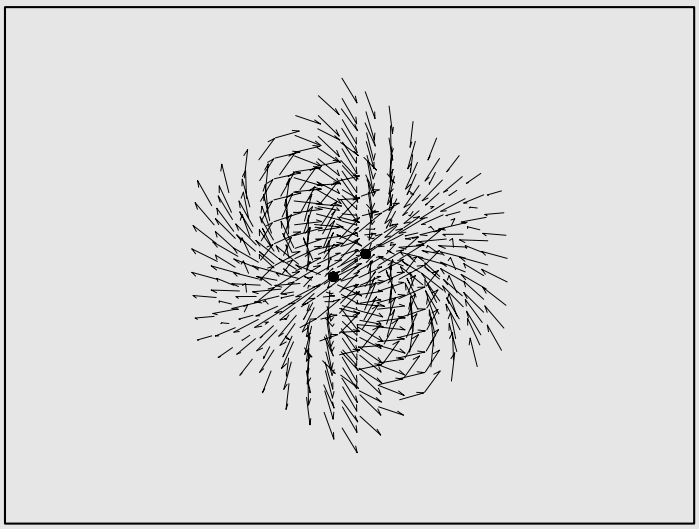
Warning, the name changecoords has been redefined

Warning, the name arrow has been redefined
```

```
> Efield := Gradient(-V,[x, y, z]);
```

$$Efield := \left(\frac{2\,x-2}{2\,(x^2-2\,x+1+y^2+z^2)^{(3/2)}}-\frac{2\,x+2}{2\,(x^2+2\,x+1+y^2+z^2)^{(3/2)}}\right)\bar{\mathbf{e}}_{\mathbf{x}} + \left(\frac{y}{(x^2-2\,x+1+y^2+z^2)^{(3/2)}}-\frac{y}{(x^2+2\,x+1+y^2+z^2)^{(3/2)}}\right)\bar{\mathbf{e}}_{\mathbf{y}} + \left(\frac{z}{(x^2-2\,x+1+y^2+z^2)^{(3/2)}}-\frac{z}{(x^2+2\,x+1+y^2+z^2)^{(3/2)}}\right)\bar{\mathbf{e}}_{\mathbf{z}}$$

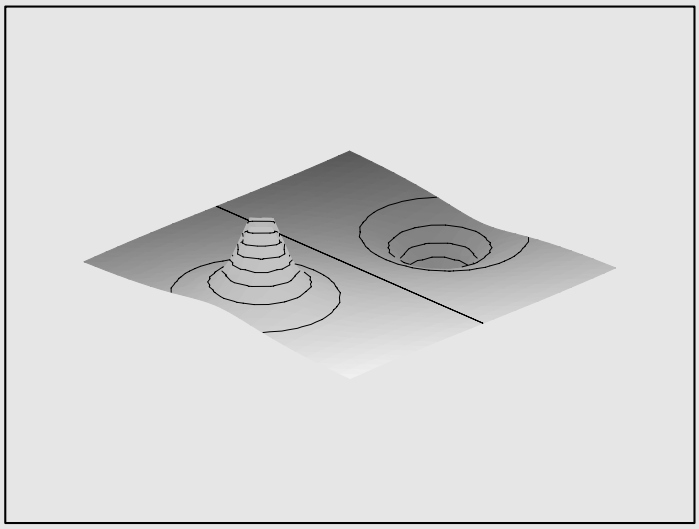
```
> fieldplot3d([Efield[1], Efield[2], Efield[3]], x=-1.5..1.5,
> y=-1.5..1.5, z=-1.5..1.5):
> NormEfield := Normalize(Efield, 2):
> p1 := sphere([1,0,0], 1/5, color=red):
> p2 := sphere([-1,0,0], 1/5, color=black):
> p3 := fieldplot3d(NormEfield, x=-4.5..4.5, y=-4.5..4.5,
> z=-4.5..4.5, color=black):
> display([p1, p2, p3], scaling=constrained);
```



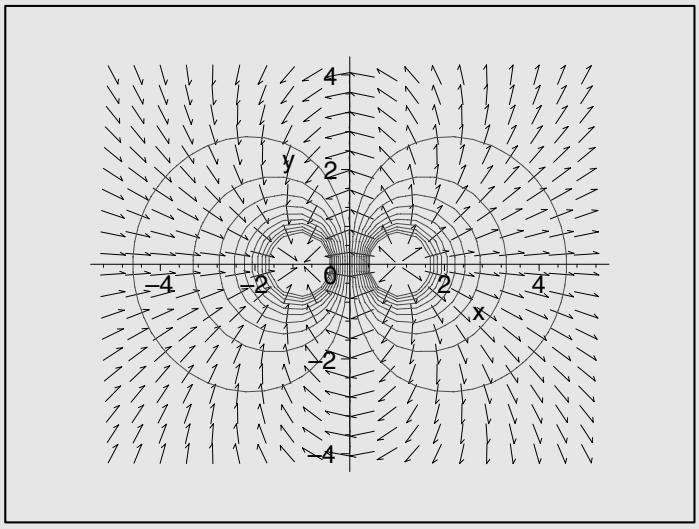
```
> z := 0;
```

$$z := 0$$

```
> plot3d(V, x=-1.5..1.5, y=-1.5..1.5, style=patchcontour,
> contours=10);
```



```
> p4 := implicitplot({seq(V=b/10, b=-10..10)}, x=-5..5, y=-4..4):
> p5 := fieldplot([NormEfield[1], NormEfield[2]], x=-5..5,
y=-4..4):
> display([p4, p5], scaling=constrained);
```



We can represent the electric field with small arrows: at any point, an arrow indicates the direction and magnitude of a vector. Such a plot is suppressed because to display the length of each arrow makes the plot difficult to understand: the range of magnitudes of $\mathbf{E}$ is usually large. In the graph shown, we have normalized those vectors which indicate only the direction of the field. We also plot the potential in the xy plane, for which the height is $V(x, y, 0)$; the

contours are lines of equipotential. When we make a plot projected in the xy plane, we see that field lines and equipotential lines are orthogonal to each other. One should be cautioned not to assume that $E_z = 0$ in the field plot in the xy plane, which cannot be shown in a two-dimensional slice.

Exercises

1. Calculate the electric field at a distance z above the center of a square of side a carrying a uniform line charge density λ along its edges.

2. Calculate the electric field on the z axis produced by a circular wire of radius R on the xy plane with line charge density $\lambda = k\cos\phi$.

3. Verify that the electric field at a distance h above the center of a rectangle on the xy plane described by $-a \le x \le a$ and $-b \le y \le y$, carrying a uniform surface charge density σ is

$$\mathbf{E} = \frac{\sigma}{\pi\epsilon_0}\tan^{-1}\left[\frac{ab}{h\sqrt{a^2+b^2+h^2}}\right]\hat{\mathbf{z}}.$$

   Hint: it might be necessary to manually manipulate the result from Maple, using $\tanh^{-1} x = -i\tan^{-1}(ix)$.

4. Calculate the electric field at a distance h above the center of a circular disk of radius R that carries a total charge Q with a surface charge density density linearly proportional to the radial distance from the center.
   Answer:

$$\mathbf{E} = \frac{3Qh}{4\pi\epsilon_0 R^3}\left[\ln\frac{R+\sqrt{R^2+h^2}}{h} - \frac{R}{\sqrt{R^2+h^2}}\right].$$

5. Find the electric field at a distance z from the center of a spherical surface of radius R that carries a uniform charge density σ; treat the cases $z < R$ and $z > R$.
   Hint: $da_2 = R^2\sin\theta_2 d\theta_2 d\phi_2$; compare the result with equation (6.42).

6. Suppose that the force between two charges takes the form

$$\mathbf{F} = \frac{kq_1q_2e^{-\mu r}}{r^2}(1+\mu r)\mathbf{e}_{12}. \tag{6.56}$$

   (a) Verify that the potential due to a point charge q_2 is

$$V(r) = \frac{kq_2e^{-\mu r}}{r}; \tag{6.57}$$

   this is a potential of Yukawa form.

(b) Referring to Figure 6.4, what is the charge residing on the inner shell in Cavendish's apparatus under this proposed force law?

7. A charge Q is distributed uniformly along a line on the z axis from $z = 0$ to $z = a$. Find the electric potential as a multipole expansion.

8. A circular disk of radius R carrying surface charge density

$$\sigma(\mathbf{r}_2) = \frac{Q}{2\pi R\sqrt{R^2 - r_2^2}}.$$

Find the electric potential as a multipole expansion.

9. An uncharged metal sphere of radius a is placed in a uniform electric field E_0 in the z direction. The induced charge distorts the field in the neighborhood of the sphere, and the potential outside the sphere is given as[5]

$$V(x, y, z) = -E_0 \left(z - \frac{a^3}{r^3} \right), \tag{6.58}$$

where $r = \sqrt{x^2 + y^2 + z^2}$. Using the method introduced in Section 6.5, take the gradient of this potential to find the electric field. Set a and E_0 to unity, and employ the `fieldplot` command to represent the electric field with small arrows; one should obtain Figure 6.7.

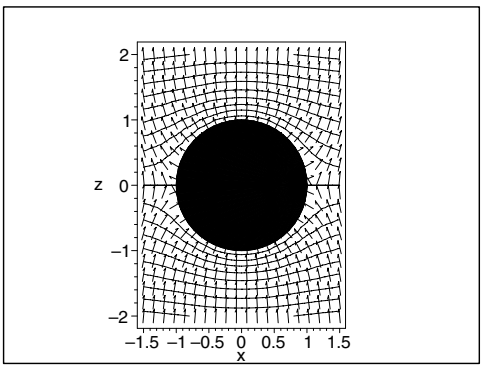


Figure 6.7: An uncharged metal sphere placed in a uniform electric field.

10. One charge $q_1 = +3$ is situated at $(1, 0, 0)$, and another charge $q_2 = -1$ is situated at $(-1, 0, 0)$. Calculate the electric potential and field. Make a plot of equipotentials and field projected in the xy plane.

11. Four electric charges have the same magnitude, two carrying positive charge situated at $(1, 1, 0)$ and $(-1, -1, 0)$, and another two carrying negative charge at $(1, -1, 0)$ and

[5] Griffiths 1999, p. 142.

$(-1, 1, 0)$. Calculate the electric potential and field. Make a plot of equipotentials and field projected in the xy plane for this electric quadrupole.

12. According to quantum mechanics to be discussed in Chapter 16, the electronic charge of a hydrogen atom in the ground state is distributed with a charge density

$$\rho(\mathbf{r}_2) = \frac{q}{\pi a_0^3} e^{-2r_2/a_0}, \tag{6.59}$$

where a_0 is the Bohr radius. To calculate the potential, we use equations (6.33) and (6.47). Because of spherical symmetry, we only have the monopole term. For an extended source, the potential is split into two parts:

$$V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0}\left[\int_0^{r_1} \frac{1}{r_1}\rho(\mathbf{r}_2) 4\pi r_2^2\, dr_2 + \int_{r_1}^{\infty} \frac{1}{r_2}\rho(\mathbf{r}_2) 4\pi r_2^2\, dr_2\right]; \tag{6.60}$$

the former for $r_1 \geq r_2$ and the latter for $r_1 \leq r_2$. Evaluate this integral to prove that

$$V(\mathbf{r}_1) = \frac{q}{4\pi\epsilon_0 r_1}\left(1 - e^{-2r_1/a_0}\right) - \frac{q}{4\pi\epsilon_0 a_0} e^{-2r_1/a_0}. \tag{6.61}$$

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7 Boundary-value Problems

The Laplacian operator appears in diverse branches of physics: in heat flow, fluid dynamics, quantum mechanics, just to name a few, in addition to electrostatics. Any function satisfying the Laplace equation is called a harmonic function. In mathematics, the Laplace equation plays a major role in the theory of analytic functions. Harmonic functions are closely related to special functions, which are well defined in Maple. In this chapter, we introduce the techniques for boundary-value problems in electrostatics.

7.1 Theory of Potential

An electric field in static conditions conforms to two of Maxwell's equations,

$$\nabla \times \mathbf{E} = 0, \tag{7.1}$$

and

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}; \tag{7.2}$$

the latter is Gauss's law. The fact that the curl of an electric field is always zero enables one to write an electric field as the gradient of a scalar function,

$$\mathbf{E} = -\nabla V, \tag{7.3}$$

where V is the electric potential. Inserting this formula into Gauss's law, we obtain

$$\nabla^2 V = -\frac{1}{\epsilon_0}\rho, \tag{7.4}$$

which is called the Poisson equation. Our objective is to solve this partial differential equation to find the potential. Once the potential is found, we can determine the electric field in space, then the force, energy, and so forth. The solution of the Poisson equation is

$$V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(\mathbf{r}_2)}{r_{12}} d\tau_2. \tag{7.5}$$

Other than for some special situations described in the preceding chapter, it is difficult to obtain the potential from this integral. In many situations, we lack the knowledge of the

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charge distribution in advance. For instance, in a metal, electric charge is freely mobile and we have no control over its distribution.

If a region of interest contains no charge, the Poisson equation becomes the Laplace equation,

$$\nabla^2 V = 0. \tag{7.6}$$

In most experiments, we maintain an electric potential difference at the boundary of a region to generate an electric field. Problems of finding the potential from given boundary conditions constitute the theory of potential.

The Laplace equation is a partial differential equation. From what we have learned in Chapter 2 on ordinary differential equations, we can obtain a general solution with undetermined coefficients; we require initial conditions to evaluate those coefficients. Similarly, general solutions of the Laplace equation for certain configurations are well studied special functions. To determine the required coefficients we need to provide boundary conditions, which are typically defined by our experimental arrangement.

The uniqueness theorem states that if the boundary conditions are specified, V is uniquely determined. Because finding the solution to the Laplace equation often involves guesswork, as we will see in many examples in this chapter, the uniqueness theorem has tremendous practical value: if we find a solution that satisfies the given boundary conditions, it is *the* solution.

7.2 Method of Images

No matter how we find a solution, as long as it satisfies the required boundary conditions, it is the only solution. The method of images is a direct application of the uniqueness theorem. If we have one or more point charges in the presence of a grounded conductor as a boundary, we can place charges of appropriate magnitude *external* to the region of interest to simulate the required boundary conditions. These charges are called image charges.

Example 7.1 A point charge q is situated a distance b away from the center of a grounded conducting sphere of radius a. Find the potential outside the sphere.

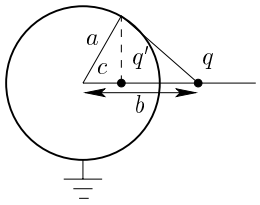


Figure 7.1: A point charge q outside a grounded conducting sphere.

Solution We place an image charge q' inside the sphere; see Figure 7.1. Note that this placement does not alter the physical condition outside, which is the region of our interest. It is convenient to place charges on the x axis; q is at $(b, 0, 0)$ and q' at $(c, 0, 0)$, where $b > a$ and $c < a$. According to such an arrangement, the potential is

$$V = \frac{1}{4\pi\epsilon_0}\left[\frac{q}{\sqrt{(x-b)^2+y^2+z^2}} + \frac{q'}{\sqrt{(x-c)^2+y^2+z^2}}\right].$$

Remember that only the region outside the sphere is of interest. Because the conducting sphere is grounded, its potential is zero. Our choice has to meet the requirement that

$$0 = \frac{1}{4\pi\epsilon_0}\left[\frac{q}{\sqrt{(a-b)^2}} + \frac{q'}{\sqrt{(a-c)^2}}\right].$$

From the geometry, the image point is at

$$bc = a^2.$$

Solving the above two equations simultaneously, we obtain

$$c = \frac{a^2}{b}, \quad q' = -\frac{a}{b}q.$$

Equipotential lines are a collection of $V =$ constant at various values, see the discussion in Section 6.5.

Worksheet 7.1 The calculations are straightforward. To plot equipotential lines, we employ the `implicitplot` command, together with the `seq` command, to generate several contours. This method will be repeatedly used in making plots in this chapter. We bring the `contourplot` command, which performs a similar function, to the reader's attention; invoke `help` for additional information.

```
> V := q1/sqrt((x-b)^2 + y^2 + z^2) + q2/sqrt((x-c)^2 + y^2 + z^2);
```

$$V := \frac{q1}{\sqrt{x^2 - 2\,x\,b + b^2 + y^2 + z^2}} + \frac{q2}{\sqrt{x^2 - 2\,x\,c + c^2 + y^2 + z^2}}$$

```
> Eq1 := eval(V, {x=a, y=0, z=0}) = 0;
```

$$Eq1 := \frac{q1}{\sqrt{a^2 - 2\,a\,b + b^2}} + \frac{q2}{\sqrt{a^2 - 2\,a\,c + c^2}} = 0$$

```
> Eq2 := b*c = a*a;
```

$$Eq2 := b\,c = a^2$$

```
> Soln1 := solve({Eq1, Eq2}, {q2, c});
```

$$Soln1 := \left\{c = \frac{a^2}{b},\ q2 = -\frac{q1\sqrt{\dfrac{a^2\,(b-a)^2}{b^2}}}{\sqrt{(b-a)^2}}\right\}$$

```
> assign(Soln1);
> V := eval(V, {b=1.5, a=1, q1=1});
```

$$V := \frac{1}{\sqrt{x^2 - 3.0\,x + 2.25 + y^2 + z^2}} - \frac{0.6666666666}{\sqrt{x^2 - 1.333333333\,x + 0.4444444444 + y^2 + z^2}}$$

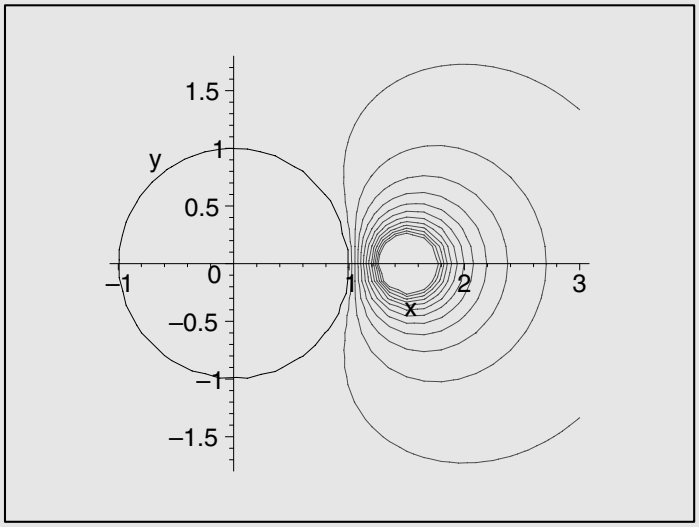
```
> with(plots):

Warning, the name changecoords has been redefined

> z := 0;
```

$$z := 0$$

```
> p1 := implicitplot({seq(V=0.25*i, i=1..12)}, x=-3..3, y=-3..3,
> scaling=constrained, numpoints=1600):
> p2 := implicitplot(V=0, x=-3..3, y=-3..3, scaling=constrained,
> color=black, thickness=2):
> display([p1, p2]);
```



After we have obtained the potential, we can calculate the electric field by taking the gradient of it, which we leave as an exercise.

7.3 Complex-variable Techniques

Some electrostatic problems in two dimensions can be solved by the use of functions of a complex variable. To avoid a rigorous mathematical treatment of complex analysis and conformal mapping, we adopt an inverse approach: we first write an answer, then find a question

that goes with it. Although this approach seems indirect, the uniqueness theorem makes this method legitimate.

A complex variable z is defined as

$$z = x + iy,$$

where x and y are real (do not confuse z with the z coordinate, which is irrelevant in two-dimensional problems). We use z as a single complex variable, and with it write ordinary mathematical functions $F(z)$; for example,

$$F(z) = z^2,$$

or

$$F(z) = \sin z.$$

In the former case we substitute $z = x + iy$ into $F(z)$, and obtain

$$F(z) = z^2 = (x + iy)^2 = x^2 - y^2 + 2ixy. \tag{7.7}$$

Thus $F(z)$ can be written as a sum of a real part and an imaginary part, each a function of x and y,

$$F(z) = u(x, y) + iv(x, y), \tag{7.8}$$

where $u(x, y)$ and $v(x, y)$ are real functions. In the above example,

$$u(x, y) = x^2 - y^2, \tag{7.9a}$$

$$v(x, y) = 2xy. \tag{7.9b}$$

Single-valued functions of a complex variable that have derivatives throughout a region of the complex plane are called *analytic functions*. We refrain from mathematical details, but understand that most "ordinary functions" (e.g., z^n, $\sin(z)$, e^z, etc.) are analytic, and their real and imaginary parts satisfy these important relations,

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \tag{7.10a}$$

$$\frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}, \tag{7.10b}$$

known as the Cauchy–Riemann equations. It follows directly that each function u or v satisfies the Laplace equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0, \tag{7.11a}$$

$$\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} = 0. \tag{7.11b}$$

To summarize the complex-variable techniques, we begin with an ordinary function $F(z)$, then we arrive at two functions $u(x, y)$ and $v(x, y)$ which both automatically constitute solutions of the Laplace equation in two dimensions. As a bonus, for a potential $u(x, y)$, the curves $v(x, y) =$ constant are field lines orthogonal to equipotential lines, and vice versa. We illustrate this method by the following example.

Example 7.2 For a function

$$F(z) = \frac{1}{z}, \tag{7.12}$$

find its real and imaginary parts, and plot $u(x, y)$ and $v(x, y)$.

Solution It is a trivial task to show that

$$u(x, y) = \Re\{f(z)\} = \frac{x}{x^2 + y^2}, \tag{7.13a}$$

$$v(x, y) = \Im\{f(z)\} = -\frac{y}{x^2 + y^2}. \tag{7.13b}$$

The symbols $\Re$ and $\Im$ denote taking the real and imaginary parts, respectively, of their operand. Letting u be the potential, we plot both $u =$ constant and $v =$ constant in the following worksheet.

Worksheet 7.2 We first declare x and y as real using `assume`. To extract real and imaginary parts, we use `Re` and `Im`, respectively; `evalc` is useful in simplifying complex expressions. Equipotentials are plotted with the `implicitplot` command as illustrated in the preceding worksheet.

```
> assume(x, real, y, real):
> z := x + I*y;
```

$$z := x + y\,I$$

```
> F := 1/z;
```

$$F := \frac{1}{x + y\,I}$$

```
> u := Re(F): u := evalc(u);
```

$$u := \frac{x}{x^2 + y^2}$$

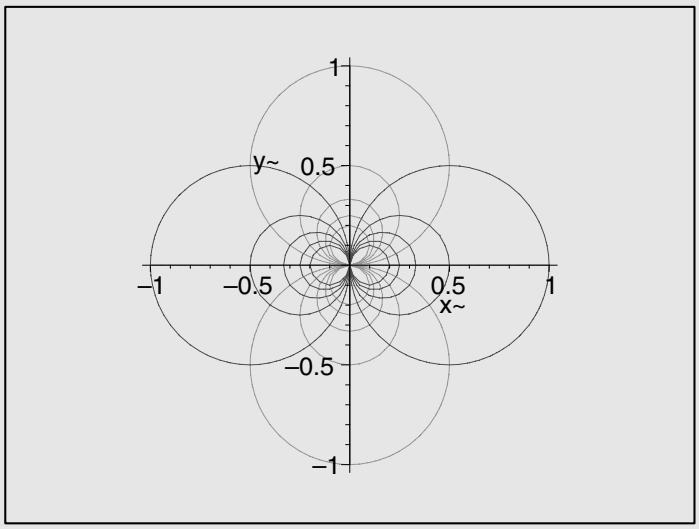
```
> v := Im(F): v := evalc(v);
```

$$v := -\frac{y}{x^2 + y^2}$$

```
> with(plots):

Warning, the name changecoords has been redefined
```

```
> p1 := implicitplot({seq(u=a, a=-5..5)}, x=-1..1, y=-1..1,
> numpoints=1600):
> p2 := implicitplot({seq(v=b, b=-5..5)}, x=-1..1, y=-1..1,
> color=green, numpoints=1600):
> display([p1, p2], scaling=constrained);
```



As we said, our approach is inverse: we write down a solution by making up functions, then we find the problem that fits that solution. From the plot, one might have guessed which problem the function u belongs to: an electric dipole in two dimensions, which can be produced by two parallel line charges with opposite polarities close together.

Consider another example,

$$F(z) = \sqrt{z}. \tag{7.14}$$

Because we have not yet learned how to take the square root of a complex variable,[1] this problem is more difficult. Nevertheless, we apply Maple to find $u(x, y)$ and $v(x, y)$ directly with the `Re` and `Im` commands:

$$u(x, y) = \Re\{F(z)\} = \left[\frac{\sqrt{x^2 + y^2} + x}{2}\right]^{1/2}, \tag{7.15a}$$

$$v(x, y) = \Im\{F(z)\} = \left[\frac{\sqrt{x^2 + y^2} - x}{2}\right]^{1/2}. \tag{7.15b}$$

[1] We can write a complex number in polar form $z = re^{i\theta}$, see Feynman 1965, vol. 2, p. 7-4.

We leave the details, which involve the handling of a "branch cut," to the reader's mathematics professor, but invoke Maple to plot $u(x, y)$ and $v(x, y)$ as shown in Figure 7.2.

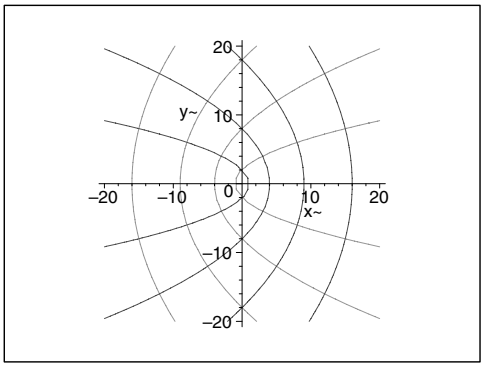


Figure 7.2: Electric field near a thin grounded plate.

Again we have a solution for which we seek a problem. Among the possible situations that this function describes, one is the potential near the edge of a grounded half-line $y = 0$, $x < 0$, for which $u =$ constant represents lines of equipotential and $v =$ constant represents field lines.

Earlier, we mentioned that harmonic functions appear in diverse branches of physics; we now digress to a different topic that requires harmonic functions. Motion of an idealized fluid in two dimensions satisfies these conditions,

$$\nabla \cdot \mathbf{V} = 0, \quad \nabla \times \mathbf{V} = 0, \tag{7.16}$$

where $\mathbf{V}$ is the velocity field. We must realize that these equations only apply to an artificial fluid, which is incompressible, nonviscous and irrotational. The mathematical structure associated with flow of an idealized fluid is entirely analogous to that of electrostatics. Because $\nabla \times \mathbf{V} = 0$, we can write the velocity as the gradient of a scalar function:

$$\nabla\phi = \mathbf{V}. \tag{7.17}$$

This scalar function ϕ is called the *velocity potential*. Apparently ϕ could be either $u(x, y)$ or $v(x, y)$ according to our complex-variable techniques above. If ϕ is chosen to be $u(x, y)$, the real part of $F(z)$, then its conjugate ψ, the complex part of $F(z)$, is the *stream function*. The lines $\psi(x, y) =$ constant are *streamlines*, which can be considered as paths of particles of the fluid.

Example 7.3 An appropriate complex potential to describe idealized flow of a fluid past a unit circular disk is

$$F(z) = z + \frac{1}{z}. \tag{7.18}$$

Find the stream function, which is the imaginary part of $F(z)$.

Solution It is straightforward to obtain

$$\psi(x,y) = \Im\{F(z)\} = y - \frac{y}{x^2+y^2}. \tag{7.19}$$

Although not formally introduced, we encourage the reader to write z in polar form as $z = re^{i\theta}$ in Maple, and to verify that

$$\psi(r,\theta) = \Im\{F(z)\} = r\sin\theta - \frac{\sin\theta}{r}. \tag{7.20}$$

A plot of several streamlines made of $\psi(x,y) =$ constant outside a unit circle $|z| = 1$ appears in the worksheet below.

Worksheet 7.3 Complex-variable techniques in fluid dynamics are identical to those in electrostatics: see the preceding worksheet. Because our interest is a region $|z| > 1$, we place a `disk`, available in the `plottools` package, in the plot to block the interior of the unit circle.

```
> assume(x, real, y, real);
> z := x + I*y;
```

$$z := x + y\,I$$

```
> F := z + 1/z;
```

$$F := x + y\,I + \frac{1}{x + y\,I}$$

```
> u := Re(F);
```

$$u := x + \frac{x}{x^2+y^2}$$

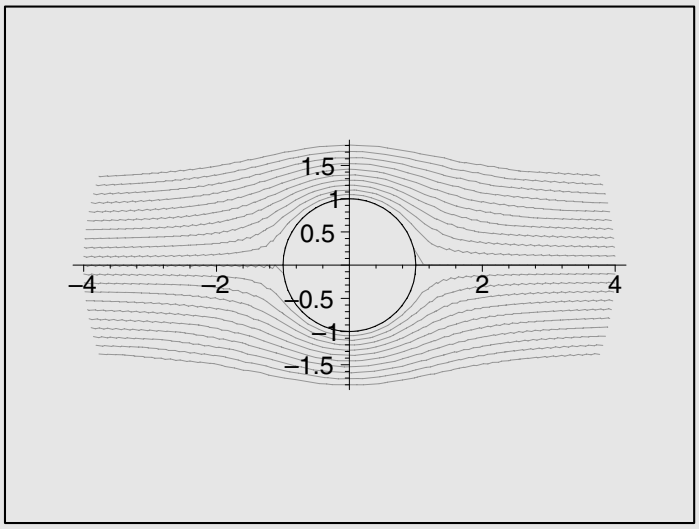
```
> v := Im(F);
```

$$v := y - \frac{y}{x^2+y^2}$$

```
> with(plots):  with(plottools):

Warning, the name changecoords has been redefined

Warning, the name arrow has been redefined
> p1 := disk([0,0], 1, color=black):
> p2 := implicitplot({seq(v=b/8, b=-10..10)}, x=-4..4, y=-2..2,
> color=black):
> display([p2, p1], scaling=constrained);
```



This plot illustrates the flow of an ideal fluid past a circular obstacle.

7.4 Laplace Equation in Cartesian Coordinates

Techniques in the preceding two sections only apply to certain situations; in this and the next two sections, we introduce a more systematic approach to the boundary-value problems. In Cartesian coordinates, the Laplace equation is

$$\nabla^2 V = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = 0. \tag{7.21}$$

The theory of potential allows us to solve for V from given boundary conditions. After we obtain the potential, we can find the electric field by calculating the gradient of the potential,

$$-\mathbf{E} = \nabla V = \frac{\partial V}{\partial x}\hat{\mathbf{x}} + \frac{\partial V}{\partial y}\hat{\mathbf{y}} + \frac{\partial V}{\partial z}\hat{\mathbf{z}}. \tag{7.22}$$

To solve the Laplace equation in multiple coordinates, which is a partial differential equation, the most intuitive method is the separation of variables. To proceed with our discussion, we must impose specific boundary conditions on the potential. Here is an illustrative example with a two-dimensional situation.

Example 7.4 Four long metallic plates form a shaft along the z direction; two of them are grounded at $y = 0$ and $y = a$, and the other two are maintained at a constant potential V_0 at $x = \pm b$; see Figure 7.3. Find the potential inside the shaft. This problem is taken from Griffiths 1999, p. 132, example 3.4.

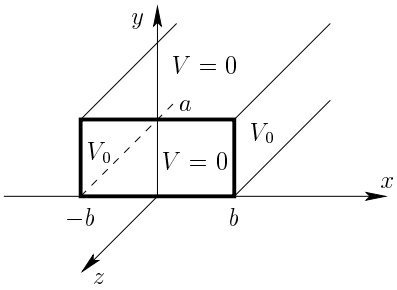


Figure 7.3: A shaft formed by four plates.

Solution We assume that V is independent of z; the Laplace equation becomes

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = 0, \tag{7.23}$$

subject to boundary conditions,

$$\begin{cases} V = 0 \text{ when } y = 0, \\ V = 0 \text{ when } y = a, \\ V = V_0 \text{ when } x = b, \\ V = V_0 \text{ when } x = -b. \end{cases} \tag{7.24}$$

The method of separation of variables involves writing the potential as a product of two functions,

$$V(x, y) = X(x)Y(y). \tag{7.25}$$

Inserting this into the Laplace equation, and dividing the equation by V, we have

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}. \tag{7.26}$$

Because each side of this equality contains a function of a separate variable, each side must be equal to a constant. We define this separation constant as k^2 to obtain two ordinary differential equations,

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = k^2, \tag{7.27}$$

$$\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = -k^2. \tag{7.28}$$

The reason we choose the constant k^2 is from hindsight: we know from experience that such a choice yields solutions in a convenient form. An alternative choice is possible, but typically produces less compact expressions. The solution of a second-order differential equation of

this type is a linear combination of sinusoidal and exponential functions. From symmetry consideration of the boundary conditions, Y must be a sine function so that it fulfils the requirements $Y(0) = 0$ and $Y(a) = 0$. For X, because it is symmetric with respect to x, a possible combination of exponential functions is the hyperbolic cosine. Therefore,

$$Y = A\sin(ky), \quad X = B\cosh(kx). \tag{7.29}$$

Our choice of these functions arises, we emphasize, from experience: one can only attain it after much practice in solving problems.

By rejecting the cosine term, we have already imposed the condition that $Y(0) = 0$; to make $Y(a) = 0$, the constant k must satisfy the following condition,

$$A\sin(ka) = 0, \quad k = \frac{n\pi}{a}, \tag{7.30}$$

where n is an integer.

We thus write the potential as

$$V = C\cosh\left(\frac{n\pi x}{a}\right)\sin\left(\frac{n\pi y}{b}\right), \tag{7.31}$$

where C is a combination of A and B.

Because n can be an arbitrary integer, V must be a linear combination of solutions of all possible n,

$$V = \sum_{n=1}^{\infty} C_n\cosh\left(\frac{n\pi x}{a}\right)\sin\left(\frac{n\pi y}{b}\right). \tag{7.32}$$

Using the boundary condition that $X(b) = V_0$, we have

$$V(b, y) = \sum_{n=1}^{\infty} C_n\cosh\left(\frac{n\pi b}{a}\right)\sin\left(\frac{n\pi y}{b}\right) = V_0. \tag{7.33}$$

This expression is simply a Fourier series; to determine C_n, we must evaluate the Fourier coefficients, a procedure described in Chapter 5:

$$C_n = \frac{2}{b}\frac{1}{\cosh(n\pi a/b)}\int_0^b V_0\sin\left(\frac{n\pi y}{b}\right)dy. \tag{7.34}$$

Worksheet 7.4 For graphical purpose, we set V_0, a and b to numerical values. Expanding a function in the Fourier series and evaluating the coefficients are the subject of numerous worksheets in Chapter 5; in this worksheet we retain nine terms. After obtaining the potential, we calculate the electric field by taking the gradient of the potential.

```
> V0:=1; a:=1; b:=1;
```

$$V0 := 1$$
$$a := 1$$
$$b := 1$$

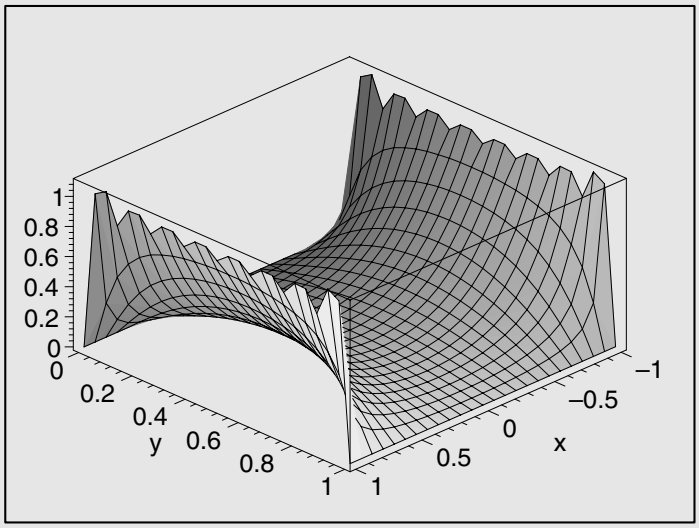
```
> kx := 2*Pi/(2*a); ky := 2*Pi/(2*b);
```

$$kx := \pi$$
$$ky := \pi$$

```
> N:=15:
> for n from 1 to N do
> C[n] := 2/(b*cosh(n*Pi*a/b))*simplify(int(V0*sin(n*ky*y),
> y=0..b));
> end do:
> V := add(C[n]*cosh(n*kx*x)*sin(n*ky*y), n=1..N);
```

$$V := \frac{4\cosh(\pi x)\sin(\pi y)}{\cosh(\pi)\pi} + \frac{4}{3}\frac{\cosh(3\pi x)\sin(3\pi y)}{\cosh(3\pi)\pi} + \frac{4}{5}\frac{\cosh(5\pi x)\sin(5\pi y)}{\cosh(5\pi)\pi}$$
$$+ \frac{4}{7}\frac{\cosh(7\pi x)\sin(7\pi y)}{\cosh(7\pi)\pi} + \frac{4}{9}\frac{\cosh(9\pi x)\sin(9\pi y)}{\cosh(9\pi)\pi}$$
$$+ \frac{4}{11}\frac{\cosh(11\pi x)\sin(11\pi y)}{\cosh(11\pi)\pi} + \frac{4}{13}\frac{\cosh(13\pi x)\sin(13\pi y)}{\cosh(13\pi)\pi}$$
$$+ \frac{4}{15}\frac{\cosh(15\pi x)\sin(15\pi y)}{\cosh(15\pi)\pi}$$

```
> plot3d(V, x=-a..a, y=0..b, axes=boxed);
```



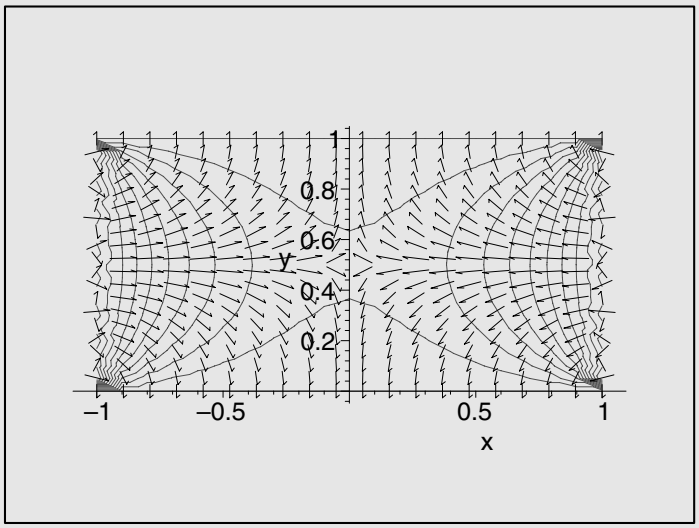
```
> with(plots): with(LinearAlgebra): with(VectorCalculus):

Warning, the name changecoords has been redefined

Warning, the names CrossProduct and DotProduct have been rebound

Warning, the assigned names <,> and <|> now have a global binding

Warning, these protected names have been redefined and unprotected: *,
+, ., Vector, diff, int, limit, series
> Efield := simplify(Gradient(-V, [x, y])):
> NormEfield := Normalize(Efield, 2): #take a while
> p1 := fieldplot([NormEfield[1], NormEfield[2]], x=-a..a, y=0..b):
> p2 := implicitplot({seq(V=b/10, b=0..10)}, x=-a..a, y=0..b,
> numpoints=400):
> display([p1, p2], scaling=constrained);
```



We show the equipotential lines on the xy plane, with the direction of the electric field. The method of producing such a plot is described in Section 6.5.

7.5 Laplace Equation in Spherical Coordinates

For expression of differential operators in spherical coordinates, Maple is resourceful. We obtain the Laplacian operator and gradient in spherical coordinates using the `VectorCalculus` package.

Worksheet 7.5

```
> with(VectorCalculus):

Warning, the assigned names <,> and <|> now have a global binding

Warning, these protected names have been redefined and unprotected: *,
+, ., Vector, diff, int, limit, series
> expand(Laplacian( V(r, theta, phi), 'spherical'[r, theta, phi]));
```

$$\frac{2\,(\frac{\partial}{\partial r}\,\mathrm{V}(r,\,\theta,\,\phi))}{r}+(\frac{\partial^2}{\partial r^2}\,\mathrm{V}(r,\,\theta,\,\phi))+\frac{\cos(\theta)\,(\frac{\partial}{\partial \theta}\,\mathrm{V}(r,\,\theta,\,\phi))}{r^2\sin(\theta)}+\frac{\frac{\partial^2}{\partial \theta^2}\,\mathrm{V}(r,\,\theta,\,\phi)}{r^2}+\frac{\frac{\partial^2}{\partial \phi^2}\,\mathrm{V}(r,\,\theta,\,\phi)}{r^2\sin(\theta)^2}$$

```
> Gradient( V(r, theta, phi), 'spherical'[r, theta, phi]);
```

$$(\frac{\partial}{\partial r}\,\mathrm{V}(r,\,\theta,\,\phi))\bar{\mathbf{e}}_{\mathbf{r}}+\frac{\frac{\partial}{\partial \theta}\,\mathrm{V}(r,\,\theta,\,\phi)}{r}\bar{\mathbf{e}}_{\boldsymbol{\theta}}+\frac{\frac{\partial}{\partial \phi}\,\mathrm{V}(r,\,\theta,\,\phi)}{r\sin(\theta)}\bar{\mathbf{e}}_{\boldsymbol{\phi}}$$

With some rearrangement, the Laplace equation in spherical coordinates is written as

$$\nabla^2 V=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial V}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial V}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2 V}{\partial\phi^2}=0, \tag{7.35}$$

and the gradient operator is

$$\nabla V=\frac{\partial V}{\partial r}\hat{\mathbf{r}}+\frac{1}{r}\frac{\partial V}{\partial\theta}\hat{\boldsymbol{\theta}}+\frac{1}{r\sin\theta}\frac{\partial V}{\partial\phi}\hat{\boldsymbol{\phi}}. \tag{7.36}$$

Note that Maple expresses the gradient in both components and basis vectors; the overbar associated with the basis vector indicates a vector field. We know that only in Cartesian coordinates are basis vectors constant; in curvilinear coordinates, a basis vector such as $\hat{\boldsymbol{\phi}}$ depends on position. The Maple output signifies

$$\bar{\mathbf{e}}_{\boldsymbol{\phi}}\equiv\hat{\boldsymbol{\phi}}(\theta,\phi),$$

and the same applies for other basis vectors.

According to the method of the separation of variables, we write V as a product of three functions:

$$V(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi). \tag{7.37}$$

Inserting this into the Laplace equation, and dividing through by V, we obtain

$$r^2\sin^2\theta\left[\frac{1}{r^2R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{1}{r^2\sin\theta\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)\right]+\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2}=0. \tag{7.38}$$

We assign a constant m^2 to the Φ part,

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2; \tag{7.39}$$

this equation is readily solved:

$$\Phi = e^{\pm im\phi}; \tag{7.40}$$

for Φ to be single-valued, m must be an integer.

We introduce another real constant $l(l+1)$ to separate equations for Θ and R:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = l(l+1), \tag{7.41}$$

and

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \left[l(l+1) - \frac{m^2}{\sin^2\theta}\right]\Theta = 0. \tag{7.42}$$

This choice of constant, $l(l+1)$, arises again from hindsight: we know beforehand that such a choice results in simplified expressions in subsequent calculations.

Maple can solve the R equation to yield an answer

$$R = Ar^l + \frac{B}{r^{l+1}}. \tag{7.43}$$

Worksheet 7.6

```
> Eq1 := 1/R(r)*diff(r^2*diff(R(r),r),r) = l*(l+1);
```

$$Eq1 := \frac{2\,r\left(\frac{d}{dr}\mathrm{R}(r)\right) + r^2\left(\frac{d^2}{dr^2}\mathrm{R}(r)\right)}{\mathrm{R}(r)} = l\,(l+1)$$

```
> Soln1 := dsolve(Eq1, R(r));
```

$$Soln1 := \mathrm{R}(r) = _C1\; r^{(-l-1)} + _C2\; r^l$$

The equation for $\Theta(\theta)$ is customarily expressed in terms of $x = \cos\theta$. After this change of variable,

$$\Theta(\theta) = P(x), \tag{7.44}$$

the equation for $P(x)$ takes the form

$$\frac{d}{dx}\left[(1-x^2)\frac{dP}{dx}\right] + \left[l(l+1) - \frac{m^2}{1-x^2}\right]P = 0. \tag{7.45}$$

This is the generalized Legendre equation, and its solutions are well established, associated Legendre functions. Combining solutions of Θ and Φ yields spherical harmonics; we defer this topic to Section 16.2 on quantum mechanics. Here we consider a case with azimuthal symmetry, that is $m = 0$. The generalized Legendre equation reduces to

$$\frac{d}{dx}\left[(1-x^2)\frac{dP}{dx}\right] + l(l+1)P = 0. \tag{7.46}$$

As we see in Chapter 5, the solutions of this equation are Legendre polynomials P_l. The general solution of the Laplace equation with azimuthal symmetry is therefore

$$V(r,\theta) = \sum_{l=0}^{\infty}\left(A_l r^l + \frac{B_l}{r^{l+1}}\right)P_l(\cos\theta). \tag{7.47}$$

We need to be more specific about the boundary conditions in order to advance our discussion.

Example 7.5 A spherical shell of radius a with an insulating ring in the plane $z = 0$ has its upper hemisphere at potential $+V_0$ and its lower hemisphere at $-V_0$. Find the potential inside the sphere.

Solution Because our interest lies in the region inside the sphere, we reject B_l terms so that V does not diverge at the origin ($r = 0$). For a given boundary condition on the shell, described by the function $f(\theta)$, we write

$$V(a,\theta) = \sum_{l=0}^{\infty} A_l a^l P_l(\cos\theta) = f(\theta). \tag{7.48}$$

This sum signifies merely expanding a function in terms of Legendre polynomials; the coefficients can be evaluated as

$$A_l = \frac{2l+1}{2a^l}\int_0^{\pi} f(\theta)P_l(\cos\theta)\,\sin\theta\,d\theta. \tag{7.49}$$

In this example,

$$f(\theta) = \begin{cases} V_0 & 0 < \theta < \pi/2 \\ -V_0 & \pi/2 < \theta < \pi. \end{cases} \tag{7.50}$$

Let $x = \cos\theta$ and $dx = -\sin\theta d\theta$;

$$A_l = \frac{2l+1}{2a^l}\int_0^1 V_0 P_l(x)dx - \frac{2l+1}{2a^l}\int_{-1}^0 V_0 P_l(x)dx. \tag{7.51}$$

We have performed an expansion of exactly this type in Section 5.4.

Worksheet 7.7 Again we set a and V_0 to unity for graphical purpose. The evaluation of the expansion coefficients is straightforward. We use the `implicitplot` command to produce equipotentials as usual.

```
> a:=1; V0:=1;
```

$$a := 1$$
$$V0 := 1$$

```
> N:=5:

> for n from 0 to N do

> C[n] := (2*n+1)/2*simplify(int(V0*LegendreP(n,x), x=0..1)+
> int(-V0*LegendreP(n,x), x=-1..0));

> end do:

> V := add(C[n]*(r/a)^n*LegendreP(n,x), n=0..N):

> V := expand(subs(x=cos(theta), V));
```

$$V := \frac{3}{2}\, r\cos(\theta) - \frac{35}{16}\, r^3\cos(\theta)^3 + \frac{21}{16}\, r^3\cos(\theta) + \frac{693}{128}\, r^5\cos(\theta)^5 - \frac{385}{64}\, r^5\cos(\theta)^3 + \frac{165}{128}\, r^5\cos(\theta)$$

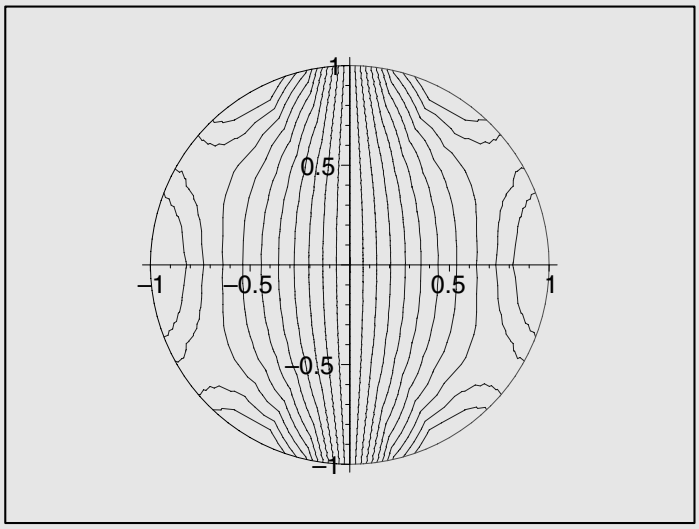
```
> with(plots):
Warning, the name changecoords has been redefined

> p1 := plot(a, theta=-Pi/2..Pi/2, coords=polar, color=red,
> thickness=2):

> p2 := plot(a, theta=Pi/2..3/2*Pi, coords=polar, color=black,
> thickness=2):

> p3 := implicitplot({seq(V=b/10, b=-10..10)}, r=0..a,
> theta=0..2*Pi, coords=polar, numpoints=800, color=blue):

> display([p1, p2, p3], scaling=constrained);
```



Because this problem has azimuthal symmetry, instead of involving three spherical coordinates, we use two polar coordinates, and plot the equipotential lines on a plane that is a cross-section of the sphere. We must be aware that in polar coordinates the angle is measured with respect to the horizontal axis, denoted by x, whereas in spherical coordinates the angle is measured with respect to the vertical axis, denoted by z. The plot that we produce above is rotated by 90° from a three-dimensional one.

7.6 Laplace Equation in Cylindrical Coordinates

Differential vector operators in cylindrical coordinates are available in Maple.

Worksheet 7.8

```
> with(VectorCalculus):

Warning, the assigned names <,> and <|> now have a global binding

Warning, these protected names have been redefined and unprotected: *,
+, ., Vector, diff, int, limit, series
> expand(Laplacian( V(rho, phi, z), 'cylindrical'[rho, phi, z]));
```

$$\frac{\frac{\partial}{\partial \rho}\mathrm{V}(\rho,\,\phi,\,z)}{\rho}+(\frac{\partial^2}{\partial \rho^2}\mathrm{V}(\rho,\,\phi,\,z))+\frac{\frac{\partial^2}{\partial \phi^2}\mathrm{V}(\rho,\,\phi,\,z)}{\rho^2}+(\frac{\partial^2}{\partial z^2}\mathrm{V}(\rho,\,\phi,\,z))$$

```
> Gradient( V(rho, phi, z), 'cylindrical'[rho, phi, z]);
```

$$(\tfrac{\partial}{\partial \rho}\,\mathrm{V}(\rho,\,\phi,\,z))\,\bar{\mathbf{e}}_{\boldsymbol{\rho}} + \frac{\frac{\partial}{\partial \phi}\,\mathrm{V}(\rho,\,\phi,\,z)}{\rho}\,\bar{\mathbf{e}}_{\boldsymbol{\phi}} + (\tfrac{\partial}{\partial z}\,\mathrm{V}(\rho,\,\phi,\,z))\,\bar{\mathbf{e}}_{\mathbf{z}}$$

The Laplace equation is

$$\nabla^2 V = \frac{\partial^2 V}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial V}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2 V}{\partial \phi^2} + \frac{\partial^2 V}{\partial z^2} = 0, \tag{7.52}$$

and the gradient is

$$\nabla V = \frac{\partial V}{\partial \rho}\hat{\boldsymbol{\rho}} + \frac{1}{\rho}\frac{\partial V}{\partial \phi}\hat{\boldsymbol{\phi}} + \frac{\partial V}{\partial z}\hat{\mathbf{z}}. \tag{7.53}$$

As customary, we employ the technique of separation of variables. Letting

$$V = R(\rho)\Phi(\phi)Z(z), \tag{7.54}$$

substituting this into the Laplace equation, dividing the result by V, and assigning two constants k and m, we obtain

$$\frac{d^2 Z}{dz^2} - k^2 Z = 0, \tag{7.55}$$

and

$$\frac{d^2 \Phi}{d\phi^2} + m^2 \Phi = 0. \tag{7.56}$$

These two equations are readily solved: Φ is a combination of sine and cosine, and Z is a combination of exponential or hyperbolic functions, depending on the boundary conditions given. The R equation is

$$\frac{d^2 R}{d\rho^2} + \frac{1}{\rho}\frac{dR}{d\rho} + \left(k^2 - \frac{m^2}{\rho^2}\right) R = 0, \tag{7.57}$$

which Maple can solve.

Worksheet 7.9

```
> Eq1 := diff(R(rho),rho$2) + 1/rho*diff(R(rho),rho) +
> (k^2-m^2/rho^2)*R(rho) = 0;
```

$$Eq1 := (\tfrac{d^2}{d\rho^2}\,\mathrm{R}(\rho)) + \frac{\frac{d}{d\rho}\,\mathrm{R}(\rho)}{\rho} + \left(k^2 - \frac{m^2}{\rho^2}\right)\mathrm{R}(\rho) = 0$$

```
> Soln1 := dsolve(Eq1, R(rho));
```

$$Soln1 := \mathrm{R}(\rho) = _C1\,\mathrm{BesselJ}(m,\,k\,\rho) + _C2\,\mathrm{BesselY}(m,\,k\,\rho)$$

The solution of the radial equation will be the Bessel functions.

We need to be more specific about the boundary conditions to advance our formulations above. As an example, consider a cylinder of radius a and height L; for the top and bottom surfaces $z = L$ and $z = 0$ respectively. The potential on the side and bottom of the cylinder is zero, and the top has a potential $V(\rho, \phi, L) = f(\rho, \phi)$; see Figure 7.4.

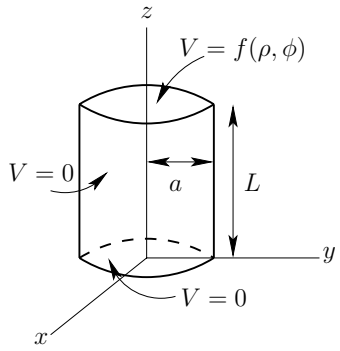


Figure 7.4: Laplace equation in cylindrical coordinates.

The solution of a problem with this configuration is

$$Z = \sinh(kz), \tag{7.58}$$

$$\Phi = A\sin(m\phi) + B(\cos m\phi), \tag{7.59}$$

$$R = CJ_m(k\rho). \tag{7.60}$$

We reject the Bessel function of the second kind $Y_m(\rho)$ because it diverges at $\rho = 0$. We choose Z and Φ in accordance with the boundary conditions.

For the potential to vanish at $\rho = a$, we must have

$$J_m(ka) = 0; \tag{7.61}$$

thus only special values are allowed for k:

$$k_{mn} = \frac{x_{mn}}{a}, \quad n = 1, 2, 3, \ldots, \tag{7.62}$$

where x_{mn} are roots of Bessel functions such that $J_m(x_{mn}) = 0$.

Combining all these conditions, we conclude that the solution in a general form is

$$V(\rho, \phi, z) = \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} J_m(k_{mn}\rho) \sinh(k_{mn}z)[A_{mn}\sin(m\phi) + B_{mn}\cos(m\phi)]. \tag{7.63}$$

This result is a Fourier series in ϕ and a Fourier–Bessel series in ρ. Because we have a boundary condition $V(\rho, \phi, L) = f(\rho, \phi)$, we write

$$f(\rho,\phi) = \sum_{m=0}^{\infty}\sum_{n=1}^{\infty} J_m(k_{mn}\rho)\sinh(k_{mn}L)[A_{mn}\sin(m\phi) + B_{mn}\cos(m\phi)]. \quad (7.64)$$

Combining the Fourier series in Section 5.1 and the Fourier–Bessel series in Section 5.5, we evaluate the coefficients as[2]

$$A_{mn} = \frac{2}{\pi a^2 J_{m+1}^2(k_{mn}a)}\frac{1}{\sinh(k_{mn}L)}\int_0^{2\pi} d\phi \int_0^a d\rho\rho f(\rho,\phi)J_m(k_{mn}\rho)\sin(m\phi), \quad (7.65)$$

$$B_{mn} = \frac{2}{\pi a^2 J_{m+1}^2(k_{mn}a)}\frac{1}{\sinh(k_{mn}L)}\int_0^{2\pi} d\phi \int_0^a d\rho\rho f(\rho,\phi)J_m(k_{mn}\rho)\cos(m\phi). \quad (7.66)$$

This result is a direct application of expansion in Bessel functions, discussed in Section 5.5.

Example 7.6 For a cylinder of radius a and height L, the potential on the side and bottom is zero, and on the top is constant, V_0. Find the potential inside the cylinder.

Solution In this problem we have azimuthal symmetry, that is $m = 0$. Therefore, we need only to expand the Fourier series in ϕ for the constant term. We remove the ϕ integral and calculate B_{0n} as

$$B_{0n} = \frac{2}{a^2 J_1^2(k_{0n}a)}\frac{1}{\sinh(k_{0n}L)}\int_0^a \rho V_0 J_0(k_{0n}\rho)\, d\rho. \quad (7.67)$$

Recall that the constant term of the Fourier coefficient is distinct from others by a factor of 2.

We find x_{0n} by numerical solutions:

$$x_{01} = 2.40, \quad x_{02} = 5.52, \quad x_{03} = 8.65, \ldots.$$

We set $L = 1$, $a = 1/2$ and $V_0 = 1$, and compute the coefficients. We have $k_{mn} = (1/a)x_{mn} = 2x_{mn}$,

$$B_{01} = \frac{2}{a^2 J_1^2(k_{01}a)}\frac{1}{\sinh(k_{01}L)}\int_0^a \rho V_0 J_0(k_{01}\rho)\, d\rho = 0.026,$$

$$B_{02} = \frac{2}{a^2 J_1^2(k_{02}a)}\frac{1}{\sinh(k_{02}L)}\int_0^a \rho V_0 J_0(k_{02}\rho)\, d\rho = -3.42\times 10^{-5},$$

$$B_{03} = \frac{2}{a^2 J_1^2(k_{03}a)}\frac{1}{\sinh(k_{03}L)}\int_0^a \rho V_0 J_0(k_{03}\rho)\, d\rho = 5.18\times 10^{-8},$$

[2]Jackson 1999, p. 118.

and so on. The potential is then written as

$$V(\rho,\phi,z) = 0.026\sinh(4.81z)J_0(4.81\rho) + 3.42\times10^{-5}\sinh(11.04z)J_0(11.04\rho) + 5.18\times10^{-8}\sinh(17.31z)J_0(17.31\rho)+\ldots.$$

Worksheet 7.10 Evaluating coefficients of expansion is similar to the content of many worksheets in this chapter. The roots for the Bessel function are retrieved using the `BesselJZeros` command. We again employ the `implicitplot` command to produce the equipotentials.

```
> x0[1] := evalf(BesselJZeros(0,1));
```

$$x0_1 := 2.404825558$$

```
> x0[2] := evalf(BesselJZeros(0,2));
```

$$x0_2 := 5.520078110$$

```
> x0[3] := evalf(BesselJZeros(0,3));
```

$$x0_3 := 8.653727913$$

```
> x0[4] := evalf(BesselJZeros(0,4));
```

$$x0_4 := 11.79153444$$

```
> x0[5] := evalf(BesselJZeros(0,5));
```

$$x0_5 := 14.93091771$$

```
> L := 1; a := 1/2; V0 := 1;
```

$$L := 1$$

$$a := \frac{1}{2}$$

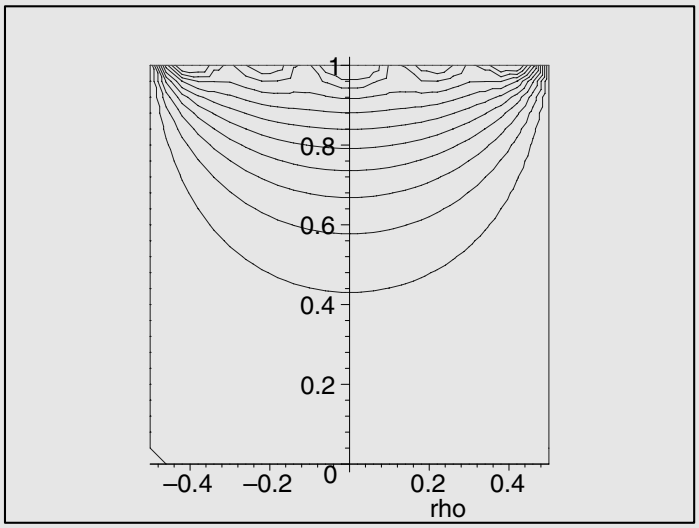
$$V0 := 1$$

```
> N := 5:
> for n from 1 to N do
> k0[n] := x0[n]/a;
> end do:
> for n from 1 to N do
> B0[n] := 2*csch(k0[n]*L)/(a^2*BesselJ(1,
> k0[n]*a)^2)*int(rho*V0*BesselJ(0, k0[n]*rho), rho=0..a);
> end do:
> V := add(B0[n]*sinh(k0[n]*z)*BesselJ(0,k0[n]*rho), n=1..N);
```

$$\begin{aligned} V := {} & 0.02611617446\sinh(4.809651116\,z)\,\mathrm{BesselJ}(0,\,4.809651116\,\rho) \\ & - 0.00003416794112\sinh(11.04015622\,z)\,\mathrm{BesselJ}(0,\,11.04015622\,\rho) \\ & + 0.5183590278\,10^{-7}\sinh(17.30745583\,z)\,\mathrm{BesselJ}(0,\,17.30745583\,\rho) \\ & - 0.8358821832\,10^{-10}\sinh(23.58306888\,z)\,\mathrm{BesselJ}(0,\,23.58306888\,\rho) \\ & + 0.1393559279\,10^{-12}\sinh(29.86183542\,z)\,\mathrm{BesselJ}(0,\,29.86183542\,\rho) \end{aligned}$$

```
> with(plots):
```

```
Warning, the name changecoords has been redefined
> p1 := plot(1, rho=-a..a, color=red, thickness=2):
> p2 := implicitplot({seq(V=b/10, b=0..10)}, rho=-a..a, z=0..L,
> color=blue):
> display([p1, p2], scaling=constrained);
```



Because this problem has azimuthal symmetry, we plot the equipotential lines on the plane of the cross-section of the cylinder.

Example 7.7 For a cylinder of radius a and height L, the potential on the side and bottom is zero, and the potential on the top is

$$V(\rho, \phi, L) = f(\rho, \phi) = \rho\,(a-\rho)\cos(3\pi\rho)\sin\phi.$$

Find the potential inside the cylinder.

Solution In this example, we must expand in both the Fourier series in ϕ and the Fourier–Bessel series in ρ; because the ϕ dependence is $\sin\phi$, only the $m = 1$ term of the Fourier series is sufficient. Therefore,

$$A_{1n} = \frac{2}{\pi a^2 J_2^2(k_{1n}a)}\frac{1}{\sinh(k_{1n}L)}\int_0^{2\pi} d\phi \int_0^a d\rho\rho[\rho\,(a-\rho)]\cos(3\pi\rho)\sin\phi J_1(k_{1n}\rho)\sin\phi. \tag{7.68}$$

The integral over ϕ yields π:

$$\int_0^{2\pi} \sin^2\phi\, d\phi = \pi.$$

Hence,

$$A_{1n} = \frac{2}{a^2 J_2^2(k_{1n}a)} \frac{1}{\sinh(k_{1n}L)} \int_0^a \rho[\rho(a-\rho)] \cos(3\pi\rho) J_1(k_{1n}\rho)\, d\rho. \tag{7.69}$$

As a numerical example to illustrate the calculations, letting $L = 1$, $a = 1/2$, we first calculate roots of the Bessel function of first order:

$$x_{11} = 3.83, \quad x_{12} = 7.02, \quad x_{13} = 10.17, \ldots.$$

We have $k_{1n} = (1/a)x_{1n} = 2x_{1n}$; the coefficients are computed as

$$A_{11} = \frac{2}{a^2 J_2^2(k_{11}a)} \frac{1}{\sinh(k_{11}L)} \int_0^a \rho[\rho(a-\rho)] \cos(3\pi\rho) J_1(k_{11}\rho)\, d\rho = -6.72 \times 10^{-5},$$

$$A_{12} = \frac{2}{a^2 J_2^2(k_{12}a)} \frac{1}{\sinh(k_{12}L)} \int_0^a \rho[\rho(a-\rho)] \cos(3\pi\rho) J_1(k_{12}\rho)\, d\rho = 9.11 \times 10^{-8},$$

$$A_{13} = \frac{2}{a^2 J_2^2(k_{13}a)} \frac{1}{\sinh(k_{13}L)} \int_0^a \rho[\rho(a-\rho)] \cos(3\pi\rho) J_1(k_{13}\rho)\, d\rho = 1.08 \times 10^{-10},$$

and so on. The potential is then

$$\begin{aligned} V(\rho,\phi,z) &= -6.72 \times 10^{-5} \sinh(7.66z) J_1(7.66\rho) \sin\phi \\ &+ 9.11 \times 10^{-8} \sinh(14.03z) J_1(14.03\rho) \sin\phi \\ &+ 1.08 \times 10^{-10} \sinh(20.35z) J_1(20.35\rho) \sin\phi + \ldots. \end{aligned}$$

Worksheet 7.11 The expansion is similar to those above. Because the potential depends on ϕ, it is difficult to plot equipotentials; we plot the potential at $z = L$ instead. To do so, we apply the `plot3d` command to produce a parametric plot in Cartesian coordinates, by setting x to be $\rho\cos\phi$ and y to be $\rho\sin\phi$.

```
> x1[1] := evalf(BesselJZeros(1,1));
```
$$x1_1 := 3.831705970$$
```
> x1[2] := evalf(BesselJZeros(1,2));
```
$$x1_2 := 7.015586670$$
```
> x1[3] := evalf(BesselJZeros(1,3));
```
$$x1_3 := 10.17346814$$
```
> x1[4] := evalf(BesselJZeros(1,4));
```
$$x1_4 := 13.32369194$$
```
> x1[5] := evalf(BesselJZeros(1,5));
```
$$x1_5 := 16.47063005$$
```
> L := 1; a := 1/2; f := rho*(a - rho)*cos(3*Pi*rho);
```
$$L := 1$$

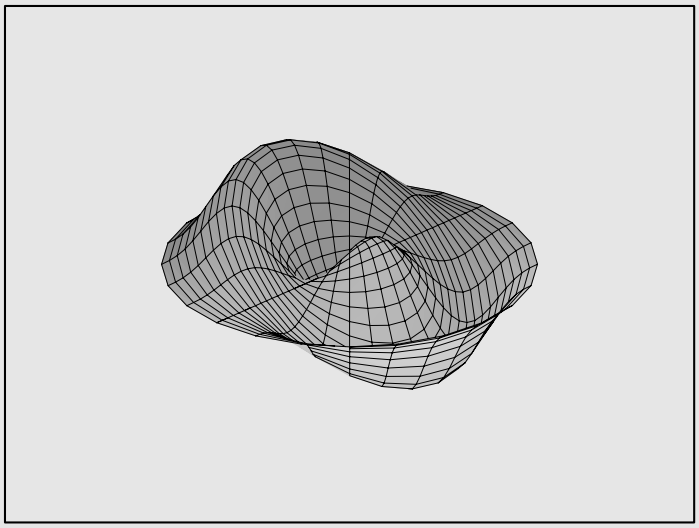
$$a := \frac{1}{2}$$

$$f := \rho \left(\frac{1}{2} - \rho \right) \cos(3\,\pi\,\rho)$$

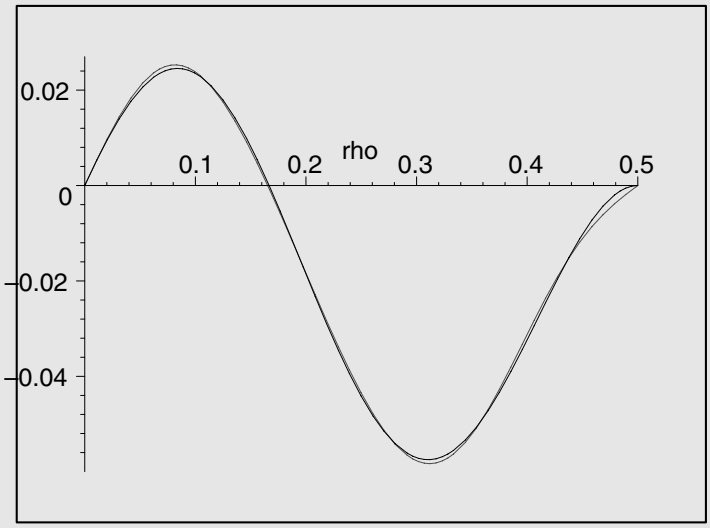
```
> N:=5:
> for n from 1 to N do
> k1[n] := x1[n]/a;
> end do:
> for n from 1 to N do
> A1[n] := evalf(2*csch(k1[n]*L)/(a^2*BesselJ(2,
> k1[n]*a)^2)*int(rho*f*BesselJ(1, k1[n]*rho), rho=0..a));
> end do:
> V := add(A1[n]*sinh(k1[n]*z)*BesselJ(1,k1[n]*rho)*sin(phi),
> n=1..N);
```

$$\begin{aligned} V := & -0.00006724668829 \sinh(7.663411940\,z)\,\mathrm{BesselJ}(1,\,7.663411940\,\rho)\sin(\phi) \\ & + 0.9105213406\,10^{-7} \sinh(14.03117334\,z)\,\mathrm{BesselJ}(1,\,14.03117334\,\rho)\sin(\phi) \\ & + 0.1075533634\,10^{-9} \sinh(20.34693628\,z)\,\mathrm{BesselJ}(1,\,20.34693628\,\rho)\sin(\phi) \\ & - 0.4924494331\,10^{-13} \sinh(26.64738388\,z)\,\mathrm{BesselJ}(1,\,26.64738388\,\rho)\sin(\phi) \\ & + 0.7131792524\,10^{-16} \sinh(32.94126010\,z)\,\mathrm{BesselJ}(1,\,32.94126010\,\rho)\sin(\phi) \end{aligned}$$

```
> plot3d([rho*cos(phi), rho*sin(phi), eval(V, z=L)], rho=0..a,
> phi=0..2*Pi);
```



```
> plot([f, eval(V, {z=L, phi=Pi/2})], rho=0..a,
> color=[black,red]);
```



As this problem entails no azimuthal symmetry, the potential is a function of three variables. It is difficult to visualize equipotential surfaces in a three-dimensional space. We make a three-dimensional plot of the potential at $z = L$, where the height is the value of the potential at this fixed z. We also construct a two-dimensional plot of the potential at $z = L$ and $\phi = \pi/2$, and compare it with the original function that describes the boundary condition; we see that the expansion satisfactorily represents the original function.

In this section, we select two particular examples so that the Fourier expansion contains only one specific value of m. In general, the ϕ dependence of the boundary condition is described with a function $g(\phi)$, which we expand in a Fourier series, and which requires extended values of m.

7.7 Summary

In most practical situations, we apply a voltage at the boundary of a region to generate an electric field within it. From given boundary conditions, we solve for the potential that satisfies the Laplace equation. We offer several worked examples of the Laplace equation in various coordinates. It is not our purpose to provide an exhaustive survey of the theory of potential; our emphasis is on computation. We apply the technique of expansion in orthogonal functions to express the potential; the coefficients are readily evaluated with Maple. One can explore

many examples from books such as Jackson 1999, or Griffiths 1999, or invent his or her own boundary conditions and express the potential in terms of special functions. Maple can perform tedious integrations, and produce graphs that allow one to verify the results.

Exercises

1. Find the electric field outside a grounded conducting sphere of radius a with a charge q at a distance b ($b > a$) from the center, which is the problem discussed in Section 7.2, and make a plot of the field.

2. Two semi-infinite grounded conducting planes meet at a right-angle. In the region between them there is a point charge q. Use the method of images to find the potential and electric field; the plot should resemble Figure 7.5

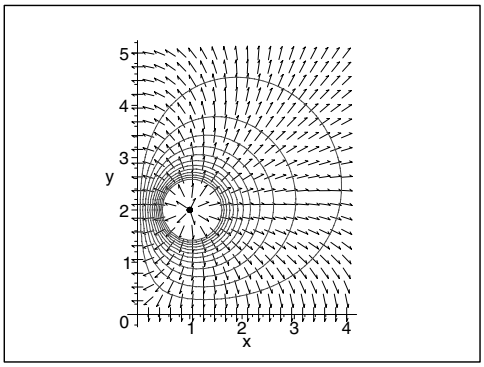


Figure 7.5: Equipotentials and field using the method of images.

3. An analytic function $F(z) = z^2$ describes many physical situations; one of them is a right-angle formed by two grounded conducting planes $x = 0$ and $y = 0$. Plot the equipotential lines using $v(x, y) = a$, and field lines using $u(x, y) = b$, for which u and v are found in equation (7.9); the graph should resemble Figure 7.6.

4. For a complex potential

$$F(z) = \ln(z + 1) - \ln(z - 1); \tag{7.70}$$

make a plot of $u(x, y) = \Re\{F(z)\} =$ constant and $v(x, y) = \Im\{F(z)\} =$ constant. Can you name a physical situation that is described by this potential?

5. Two-dimensional electric quadrupole focusing fields for particle accelerators can be modeled as a set of four symmetrically placed line charges, with line charge densities $\pm\lambda$. The electric potential is the real part of

$$F(z) = \frac{2\lambda}{4\pi\epsilon_0} \ln\left[\frac{(z - ia)(z + ia)}{(z - a)(z + a)}\right]; \tag{7.71}$$

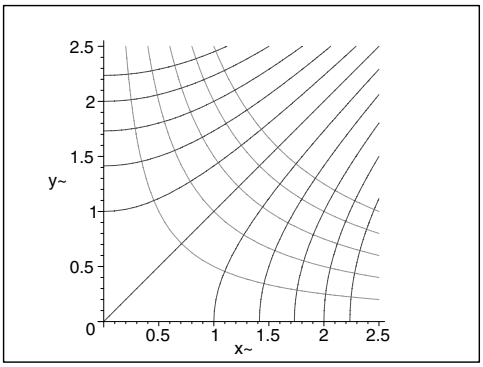


Figure 7.6: Equipotentials and field lines near the corner using complex variables.

see Jackson 1999, problem 2.20, p. 91. Make a plot of the equipotential and field lines; the graph should resemble Figure 7.7.

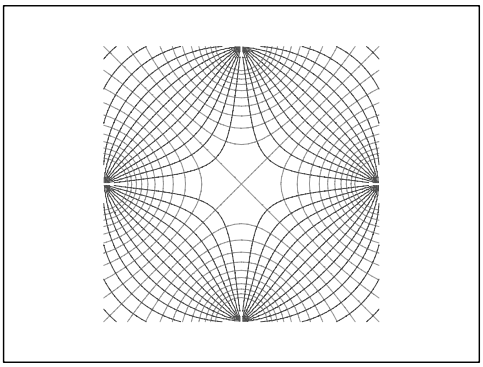


Figure 7.7: Equipotentials and field lines of quadrupole focusing fields.

6. Consider the motion of a fluid having a complex potential

$$F(z) = z + \frac{1}{z} + i\gamma \ln z, \tag{7.72}$$

for (a) $\gamma = 1.6$; (b) $\gamma = 2.8$. We have discussed the situation of $\gamma = 0$ in Section 7.3; a nonvanishing γ represents a circulation around the cylinder. Plot the streamlines, which are made of $\psi(x, y) = \Im\{F(z)\} =$ constant outside a unit circle $|z| = 1$; one should notice how the pattern of flow varies with γ, as shown in Figure 7.8.

7. In all examples within this chapter, increase the number of terms of coefficients in the expansion in orthogonal functions, and observe the output.

8. A conducting spherical shell of radius a is cut into three segments, as shown in Figure 7.9. The top ($0 \leq \theta \leq \pi/3$) and bottom ($2\pi/3 \leq \theta \leq \pi$) segments are grounded, and the

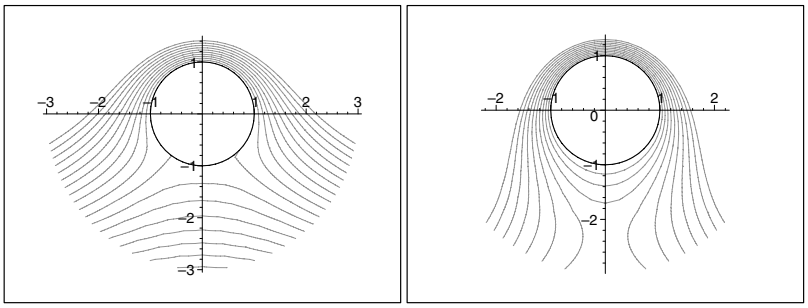


Figure 7.8: The streamlines past a circular disk in two situations.

middle segment ($\pi/3 \leq \theta \leq 2\pi/3$) is maintained at potential V_0. Find the potential inside this shell.

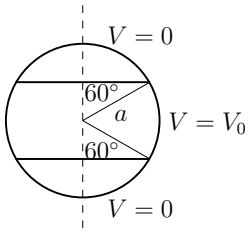


Figure 7.9: A spherical shell divided into three segments.

9. A hollow sphere of radius a is maintained at potential

$$V(a, \theta) = f(\theta) = \sin^2(\theta/2).$$

Find the potential $V(r, \theta)$ inside the sphere.

10. For a cylinder of radius a and height L, the potential on the side and bottom is zero, and for the top is

$$V(\rho, \phi, L) = f(\rho, \phi) = \rho(a-\rho)\cos(3\pi\rho)\left[\sin(\phi) + \cos(4\phi)\right].$$

Find the potential $V(\rho, \phi, z)$ inside the cylinder.

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8 Magnetostatics

In this chapter we study magnetism in a steady condition. In addition to sophisticated integrals similar to those encountered in calculating electric fields, problems regarding magnetic fields are further complicated because they typically involve a cross-product of two vectors. For instance, to calculate the magnetic force one needs to find the cross-product of the velocity of a moving charge and the magnetic field, and to calculate the magnetic field produced by a current element one needs to find the cross-product of the line element vector and the separation vector. We explore Maple's capability for vector calculus and linear algebra to solve problems of magnetostatics.

8.1 Magnetic Forces

A stationary charge in an electric field experiences a force: that is the domain of electrostatics. A moving charge q experiences an additional force for which an electric field takes no account. We define the magnetic field $\mathbf{B}$ through the total force acting on a moving charge:

$$\mathbf{F} = q[\mathbf{E} + (\mathbf{v} \times \mathbf{B})]; \tag{8.1}$$

this equation is the Lorentz force law. We understand that the magnetic force is proportional to the cross-product of velocity and magnetic field; hence equations of motion are a set of coupled differential equations. We use an example to observe the motion of a charged particle subject to both electric and magnetic fields.

Example 8.1 Suppose that we have both electric and magnetic fields in a region. The uniform electric field is in the z direction, and the uniform magnetic field is in the x direction. Find the trajectory of a charged particle, released at the origin at time 0 and initial velocity $v_{0y}\,\hat{\mathbf{y}} + v_{0z}\,\hat{\mathbf{z}}$.

Solution The Lorentz force is

$$\mathbf{F} = q[\mathbf{E} + (\mathbf{v} \times \mathbf{B})] = q\dot{z}B_x\hat{\mathbf{y}} + q(E_z - \dot{y}B_x)\hat{\mathbf{z}}. \tag{8.2}$$

Applying Newton's second law, we form three differential equations,

$$F_x = ma_x, \qquad 0 = m\ddot{x}, \tag{8.3a}$$

$$F_y = ma_y, \qquad q\dot{z}B_x = m\ddot{y}, \tag{8.3b}$$

$$F_z = ma_z, \quad q(E_z - \dot{y}B_x) = m\ddot{z}, \tag{8.3c}$$

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among which the y and z equations are coupled. The particle is released from the origin with initial velocity $v_{0y}\hat{\mathbf{y}} + v_{0z}\hat{\mathbf{z}}$; with these initial conditions, the solutions are

$$x = 0, \tag{8.4a}$$

$$y = \frac{1}{\omega B_x}[E_z\omega t - E_z \sin(\omega t) + v_{0y}B_x \sin(\omega t) + v_{0z}B_x - v_{0z}B_x(\cos\omega t)], \tag{8.4b}$$

$$z = \frac{1}{\omega B_x}[E_z - E_z \cos(\omega t) + v_{0y}B_x \cos(\omega t) - v_{0y}B_x + v_{0z} \sin(\omega t)], \tag{8.4c}$$

where ω is the cyclotron frequency,

$$\omega \equiv \frac{qB_x}{m}. \tag{8.5}$$

Worksheet 8.1 The `map` command is particularly useful for managing vectors: in this worksheet we use it to apply the `diff` operator to each component of the position vector in order to find the velocity and acceleration. Basic vector algebra operations, such as multiplication of a vector by a scalar defined as `ScalarMultiply`, and the cross-product of two vectors defined as `CrossProduct`, are implemented in the `LinearAlgebra` package. The syntax is expected to be self-explanatory; one can seek additional information from help. We invoke the `seq` command to generate a system of three differential equations; in this problem, they can be solved analytically using the `dsolve` command.

```
> with(LinearAlgebra):
> r := < x(t) | y(t) | z(t) >;
```

$$r := [\mathrm{x}(t),\ \mathrm{y}(t),\ \mathrm{z}(t)]$$

```
> v := map(diff, r, t);
```

$$v := \left[\tfrac{d}{dt}\,\mathrm{x}(t),\ \tfrac{d}{dt}\,\mathrm{y}(t),\ \tfrac{d}{dt}\,\mathrm{z}(t)\right]$$

```
> a := map(diff, v, t);
```

$$a := \left[\tfrac{d^2}{dt^2}\,\mathrm{x}(t),\ \tfrac{d^2}{dt^2}\,\mathrm{y}(t),\ \tfrac{d^2}{dt^2}\,\mathrm{z}(t)\right]$$

```
> F := ScalarMultiply(a, m);
```

$$F := \left[m\,(\tfrac{d^2}{dt^2}\,\mathrm{x}(t)),\ m\,(\tfrac{d^2}{dt^2}\,\mathrm{y}(t)),\ m\,(\tfrac{d^2}{dt^2}\,\mathrm{z}(t))\right]$$

```
> B := < Bx | 0 | 0 >;
```

$$B := [Bx,\ 0,\ 0]$$

```
> E := < 0 | 0 | Ez >;
```

$$E := [0,\ 0,\ Ez]$$

```
> Lorentz := ScalarMultiply((E + CrossProduct(v, B)), q);
```

$$Lorentz := \left[0,\ q\,(\tfrac{d}{dt}\,\mathrm{z}(t))\,Bx,\ q\,(Ez - (\tfrac{d}{dt}\,\mathrm{y}(t))\,Bx)\right]$$

```
> Epr1 := F - Lorentz;
```

$$Epr1 := \left[m\left(\frac{d^2}{dt^2}\,\mathrm{x}(t)\right),\ m\left(\frac{d^2}{dt^2}\,\mathrm{y}(t)\right) - q\left(\frac{d}{dt}\,\mathrm{z}(t)\right) Bx,\ m\left(\frac{d^2}{dt^2}\,\mathrm{z}(t)\right) - q\left(Ez - \left(\frac{d}{dt}\,\mathrm{y}(t)\right) Bx\right)\right]$$

```
> ini := x(0)=0, y(0)=0, z(0)=0, D(x)(0)=0, D(y)(0)=vy0,
> D(z)(0)=vz0;
```

$$ini := \mathrm{x}(0) = 0,\ \mathrm{y}(0) = 0,\ \mathrm{z}(0) = 0,\ \mathrm{D}(x)(0) = 0,\ \mathrm{D}(y)(0) = vy0,\ \mathrm{D}(z)(0) = vz0$$

```
> Soln1 := dsolve({seq(Epr1[i]=0, i=1..3), ini}, {x(t), y(t),
z(t)});
```

$$Soln1 := \left\{\mathrm{x}(t) = 0,\right.$$

$$\mathrm{z}(t) = \frac{m\,vz0\sin\left(\frac{Bx\,q\,t}{m}\right) Bx + m\,(-Ez + vy0\,Bx)\cos\left(\frac{Bx\,q\,t}{m}\right) + m\,Ez - m\,vy0\,Bx}{q\,Bx^2},$$

$$\left.\mathrm{y}(t) = -\frac{vz0\,m\cos\left(\frac{Bx\,q\,t}{m}\right) - \frac{(-Ez + vy0\,Bx)\sin\left(\frac{Bx\,q\,t}{m}\right) m}{Bx} - Ez\,t\,q - vz0\,m}{Bx\,q}\right\}$$

```
> Soln2 := algsubs(q*Bx/m=omega, Soln1):
> Soln3 := simplify(Soln2);
```

$$Soln3 := \left\{\mathrm{x}(t) = 0,\right.$$

$$\mathrm{z}(t) = \frac{m\,(-\cos(t\,\omega)\,Ez + \cos(t\,\omega)\,vy0\,Bx + Bx\,vz0\sin(t\,\omega) - vy0\,Bx + Ez)}{q\,Bx^2},$$

$$\left.\mathrm{y}(t) = \frac{-\sin(t\,\omega) m\,Ez + \sin(t\,\omega) m\,vy0\,Bx + Ez\,t\,q\,Bx - vz0\,m\,Bx\cos(t\,\omega) + vz0\,m\,Bx}{q\,Bx^2}\right\}$$

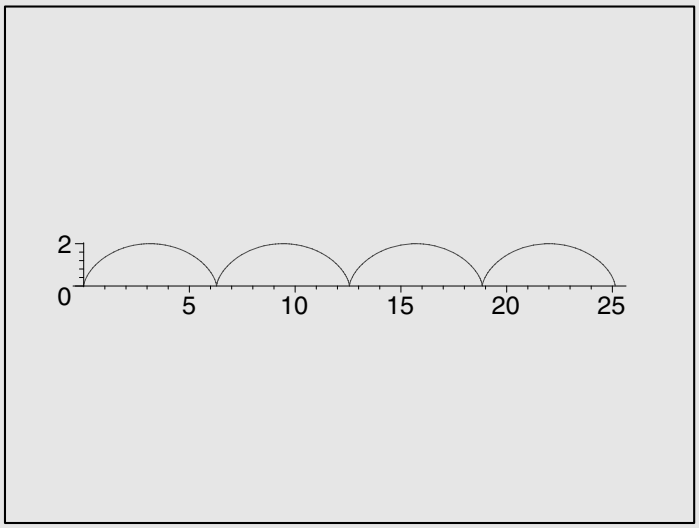
```
> m := 1;  q := 1;  Bx := 1;  Ez := 1;  vy0 := 0;  vz0 := 0;
> # one can try other vy0 and vz0.
```

$$m := 1$$
$$q := 1$$
$$Bx := 1$$
$$Ez := 1$$
$$vy0 := 0$$
$$vz0 := 0$$

```
> Soln1;
```

$$\{\mathrm{y}(t) = -\sin(t) + t,\ \mathrm{x}(t) = 0,\ \mathrm{z}(t) = 1 - \cos(t)\}$$

```
> assign(Soln1);
> plot([y(t), z(t), t=0..25], scaling=constrained);
```



After substituting in the numerical values, we plot the trajectory. This curve looks familiar: the cycloid that we encountered in the brachistochrone problem in Chapter 3. We leave to the reader as an exercise to plot trajectories with other initial conditions.

8.2 Biot–Savart Law

The electric current is defined as the charge per unit time passing a given point. A line charge λ traveling along the wire at speed v constitutes a current,

$$\mathbf{I} = \lambda \mathbf{v}. \tag{8.6}$$

When charge flows over a surface, we describe it with the surface current density $\mathbf{K}$,

$$\mathbf{K} = \sigma \mathbf{v}, \tag{8.7}$$

where σ is the surface charge density. We define, analogously, the volume current density $\mathbf{J}$ as

$$\mathbf{J} = \rho \mathbf{v}, \tag{8.8}$$

where ρ is the volume charge density. The magnetic field due to a steady current along a line is given by the Biot–Savart law,

$$\mathbf{B}(\mathbf{r}_1) = \frac{\mu_0}{4\pi} I \int \frac{d\mathbf{l}_2 \times \mathbf{e}_{12}}{r_{12}^2}. \tag{8.9}$$

The constant μ_0 is called the permeability of free space; in SI units its value is

$$\mu_0 = 4\pi \times 10^{-7}\ \mathrm{N\,A^{-2}}. \tag{8.10}$$

With SI units for length in meters (m) and electric current in amperes (A), the magnetic field has the unit tesla (T).

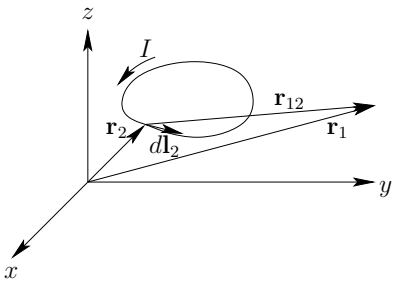


Figure 8.1: Notation for the Biot–Savart law.

Similar to our discussion for Coulomb's law, we here devote particular attention to our notation. According to Figure 8.1, $\mathbf{r}_1$ is the position vector for the *field point*, at which we intend to determine the strength of the field, $\mathbf{r}_2$ is the position vector for the *source point*, at which the current in an element of length contributes to the field, and $\mathbf{r}_{12}$ is the *separation vector*, of which the length is r_{12},

$$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2, \quad r_{12} = |\mathbf{r}_{12}|. \tag{8.11}$$

The unit vector $\mathbf{e}_{12}$ is the normalized vector of $\mathbf{r}_{12}$,

$$\mathbf{e}_{12} = \frac{\mathbf{r}_{12}}{r_{12}}. \tag{8.12}$$

Integration is performed with respect to the source; the line element $d\mathbf{l}_2$ in Cartesian coordinates is

$$d\mathbf{l}_2 = dx_2\hat{\mathbf{x}} + dy_2\hat{\mathbf{y}} + dz_2\hat{\mathbf{z}}. \tag{8.13}$$

The direction of the magnetic field is the direction of the cross-product of $d\mathbf{l}_2$ and $\mathbf{e}_{12}$. If a surface or volume current density is provided, we alter the form of the integral appropriately:

$$\mathbf{B}(\mathbf{r}_1) = \frac{\mu_0}{4\pi} \int \frac{\mathbf{K}(\mathbf{r}_2) \times \mathbf{e}_{12}}{r_{12}^2} da_2, \quad \mathbf{B}(\mathbf{r}_1) = \frac{\mu_0}{4\pi} \int \frac{\mathbf{J}(\mathbf{r}_2) \times \mathbf{e}_{12}}{r_{12}^2} d\tau_2. \tag{8.14}$$

We adopt this notation consistently so that we can apply this formulation directly in a calculation.

Example 8.2 Evaluate the magnetic field $\mathbf{B}$ at a distance s from a segment of wire carrying a steady current i.

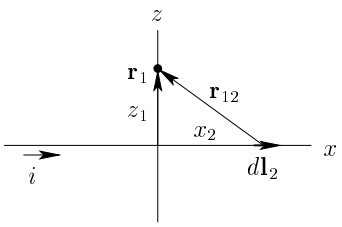


Figure 8.2: A wire carrying a steady current i.

Solution We choose the coordinate system so that the wire lies along the x axis and the field point is on the z axis:

$$\mathbf{r}_2 = x_2\hat{\mathbf{x}}, \quad \mathbf{r}_1 = z_1\hat{\mathbf{z}}.$$

We have

$$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2, \quad r_{12} = \sqrt{x_2^2 + z_1^2},$$

$$d\mathbf{l}_2 = dx_2\hat{\mathbf{x}}, \quad \mathbf{e}_{12} = \frac{-x_2}{\sqrt{x_2^2 + z_1^2}}\hat{\mathbf{x}} + \frac{z_1}{\sqrt{x_2^2 + z_1^2}}\hat{\mathbf{z}},$$

$$d\mathbf{l}_2 \times \mathbf{e}_{12} = -\frac{z_1\, dx_2}{\sqrt{x_2^2 + z_1^2}}\hat{\mathbf{y}}.$$

As all elements needed for integration of the Biot–Savart law are available, we find the magnetic field:

$$B_y = \frac{\mu_0 i}{4\pi}\int_a^b \frac{1}{x_2^2 + z_1^2}\left(-\frac{z_1\, dx_2}{\sqrt{x_2^2 + z_1^2}}\right) = \frac{\mu_0 i}{4\pi}\frac{a\sqrt{b^2 + z_1^2} - b\sqrt{a^2 + z_1^2}}{z_1\sqrt{b^2 + z_1^2}\sqrt{a^2 + z_1^2}}. \tag{8.15}$$

Worksheet 8.2 Application of the `LinearAlgebra` package in this worksheet is similar to that in Section 6.1 in which we discuss Coulomb's law. If we adopt the symbols in a clear and systematic fashion, the calculations proceed readily.

```
> assume(x2, real, z1, real):
> with(LinearAlgebra):
> r2vec := < x2 | 0 | 0 >;
                          r2vec := [x2, 0, 0]
> r1vec := < 0 | 0 | z1 >;
                          r1vec := [0, 0, z1]
```

```
> r12vec := r1vec - r2vec;
```

$$r12vec := [-x2,\ 0,\ z1]$$

```
> dl2 := map(diff, r2vec, x2);
```

$$dl2 := [1,\ 0,\ 0]$$

```
> e12 := Normalize(r12vec, 2):
> e12 := map(simplify, e12);
```

$$e12 := \left[-\frac{x2}{\sqrt{x2^2 + z1^2}},\ 0,\ \frac{z1}{\sqrt{x2^2 + z1^2}}\right]$$

```
> r12 := Norm(r12vec, 2):
> r12 := simplify(r12);
```

$$r12 := \sqrt{x2^2 + z1^2}$$

```
> Bdir := CrossProduct(dl2, e12);
```

$$Bdir := \left[0,\ -\frac{z1}{\sqrt{x2^2 + z1^2}},\ 0\right]$$

```
> By := mu[0]*i/(4*Pi)*int(Bdir[2]/r12^2, x2=a..b);
```

$$By := \frac{1}{4}\,\frac{\mu_0\, i\,(-b\sqrt{a^2 + z1^2} + a\sqrt{b^2 + z1^2})}{\pi\, z1\,\sqrt{b^2 + z1^2}\,\sqrt{a^2 + z1^2}}$$

```
> By1 := limit(By, a=-infinity):  By2 := limit(By1, b=infinity);
```

$$By2 := -\frac{1}{2}\,\frac{\mu_0\, i}{\pi\, z1}$$

For an infinitely long wire, that is $a \to -\infty$ and $b \to \infty$, the magnetic field is

$$B = -\frac{1}{2}\frac{\mu_0 i}{\pi z_1}, \tag{8.16}$$

which points to negative y; hence the direction of the magnetic field curls around the wire.

Example 8.3 Find the magnetic field $\mathbf{B}$ at a distance z above the center of a circular loop of radius R that carries a steady current i; see Figure 8.3.

Solution Spherical coordinates in Cartesian basis vectors, discussed in Section 6.2, are clearly convenient here. The position vector for a source point is

$$\mathbf{r}_2 = R\cos\phi\,\hat{\mathbf{x}} + R\sin\phi\,\hat{\mathbf{y}},$$

and that for a field point is

$$\mathbf{r}_1 = z_1\hat{\mathbf{z}};$$

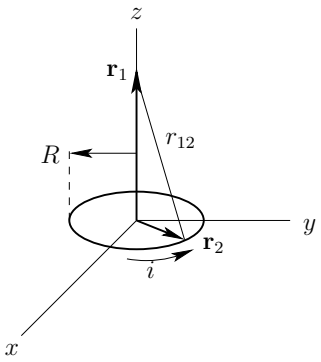


Figure 8.3: A current loop.

the length of the separation vector is

$$r_{12} = \sqrt{R^2 + z_1^2}.$$

The differential displacement is

$$d\mathbf{l}_2 = \frac{\partial \mathbf{r}_2}{\partial r} dr + \frac{\partial \mathbf{r}_2}{\partial \phi} d\phi + \frac{\partial \mathbf{r}_2}{\partial z} dz; \tag{8.17}$$

therefore,

$$d\mathbf{l}_2 = \frac{d\mathbf{r}_2}{d\phi} d\phi = -R \sin\phi \, d\phi \, \hat{\mathbf{x}} + R \cos\phi \, d\phi \, \hat{\mathbf{y}}.$$

The normalized separation vector is

$$\mathbf{e}_{12} = -\frac{R\cos\phi}{\sqrt{R^2 + z_1^2}} \hat{\mathbf{x}} - \frac{R\sin\phi}{\sqrt{R^2 + z_1^2}} \hat{\mathbf{y}} + \frac{z_1}{\sqrt{R^2 + z_1^2}} \hat{\mathbf{z}};$$

then

$$d\mathbf{l}_2 \times \mathbf{e}_{12} = \frac{z_1 R \cos\phi}{\sqrt{R^2 + z_1^2}} d\phi \, \hat{\mathbf{x}} + \frac{z_1 R \sin\phi}{\sqrt{R^2 + z_1^2}} d\phi \, \hat{\mathbf{y}} + \frac{R^2}{\sqrt{R^2 + z_1^2}} d\phi \, \hat{\mathbf{z}}.$$

Because the x and y components contain $\cos\phi$ and $\sin\phi$, respectively, the integral over ϕ through a complete cycle is zero; only the z component is nonvanishing:

$$B_z = \frac{\mu_0 i}{4\pi} \int_0^{2\pi} \frac{1}{R^2 + z_1^2} \frac{R^2}{\sqrt{R^2 + z_1^2}} d\phi = \frac{\mu_0 i}{2} \frac{R^2}{(R^2 + z_1^2)^{3/2}}. \tag{8.18}$$

As the integrand is independent of ϕ, the integration simply gives a factor of 2π.

Worksheet 8.3 We follow the convention for symbols in the preceding worksheets.

```
> assume(z1, real, R, real, phi2, real):
> with(LinearAlgebra):
> r2vec := < R*cos(phi2) | R*sin(phi2) | 0 >;
```

$$r2vec := [R\cos(\phi 2),\ R\sin(\phi 2),\ 0]$$

```
> r1vec := < 0 | 0 | z1 >;
```

$$r1vec := [0,\ 0,\ z1]$$

```
> r12vec := r1vec - r2vec;
```

$$r12vec := [-R\cos(\phi 2),\ -R\sin(\phi 2),\ z1]$$

```
> dl2 := map(diff, r2vec, phi2);
```

$$dl2 := [-R\sin(\phi 2),\ R\cos(\phi 2),\ 0]$$

```
> e12 := Normalize(r12vec, 2):
> e12 := map(simplify, e12);
```

$$e12 := \left[-\frac{R\cos(\phi 2)}{\sqrt{R^2+z1^2}},\ -\frac{R\sin(\phi 2)}{\sqrt{R^2+z1^2}},\ \frac{z1}{\sqrt{R^2+z1^2}}\right]$$

```
> r12 := Norm(r12vec, 2):
> r12 := simplify(r12);
```

$$r12 := \sqrt{R^2+z1^2}$$

```
> Bdir := CrossProduct(dl2, e12):
> Bdir := map(simplify, Bdir);
```

$$Bdir := \left[\frac{R\cos(\phi 2)\,z1}{\sqrt{R^2+z1^2}},\ \frac{R\sin(\phi 2)\,z1}{\sqrt{R^2+z1^2}},\ \frac{R^2}{\sqrt{R^2+z1^2}}\right]$$

```
> Bz := mu[0]*i/(4*Pi)*int(Bdir[3]/r12^2, phi2=0..2*Pi);
```

$$Bz := \frac{1}{2}\,\frac{\mu_0\, i\, R^2}{(R^2+z1^2)^{(3/2)}}$$

The reader is encouraged to modify the worksheet to calculate the field at a point off-axis. One might choose the field point in the xz plane (i.e., $\mathbf{r}_1 = x_1\hat{\mathbf{x}} + z_1\hat{\mathbf{z}}$) without loss of generality, and Maple should return the x and z components of the field in terms of elliptic integrals, although these results are not particularly illuminating.

Because the integral of the field involves r_{12}, the length of the separation vector, we can employ equation (6.46) to expand r_{12} in Legendre polynomials; see an exercise at the end of the chapter. Such a calculation gives a multipole expansion in magnetism. From equation (8.54), neglecting terms in r_1^{-4} and higher, we have

$$\mathbf{B} = \frac{\mu_0}{4\pi r_1^3} i\pi R^2 (2\cos\theta_1 \hat{\mathbf{r}} + \sin\theta_1 \hat{\boldsymbol{\theta}}). \tag{8.19}$$

For $z_1 \gg R$ equation (8.18) becomes

$$B_z = \frac{\mu_0}{4\pi}\frac{2i\pi R^2}{z_1^3}, \tag{8.20}$$

which is equation (8.19) at $\theta_1 = 0$. By analogy with electrostatics, we define a magnetic dipole as a system of current distribution that produces a magnetic field proportional to r^{-3}. Therefore,

$$m \equiv iA = i\pi R^2. \tag{8.21}$$

A current loop thus serves as an example of a magnetic dipole, provided $r_1 \gg R$.

8.3 Vector Potential

In electrostatics we introduce the electric potential, which is the integral of the electric field. It is often easier to calculate the potential first and then to differentiate it to evaluate the field, than it is to integrate directly from Coulomb's law. We analogously introduce the magnetic vector potential that is the integral of the magnetic field. The reason why we can represent $\mathbf{E}$ as a gradient of a scalar potential is that the curl of $\mathbf{E}$ is always zero; in contrast, in magnetostatics the curl of magnetic field $\mathbf{B}$ is not always zero. For this reason one cannot, in general, represent a magnetic field as a gradient of a scalar function. However, by Gauss's law of magnetism, the divergence of $\mathbf{B}$ is always zero,

$$\nabla \cdot \mathbf{B} = 0. \tag{8.22}$$

Hence we can represent $\mathbf{B}$ as the curl of another vector field,

$$\mathbf{B} = \nabla \times \mathbf{A}, \tag{8.23}$$

where $\mathbf{A}$ is the magnetic vector potential.

Ampère's law is

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J}; \tag{8.24}$$

the solution for the vector potential is

$$\mathbf{A}(\mathbf{r}_1) = \frac{\mu_0}{4\pi} I \int \frac{d\mathbf{l}_2}{r_{12}}, \tag{8.25}$$

or in terms of volume or area current density,

$$\mathbf{A}(\mathbf{r}_1) = \frac{\mu_0}{4\pi}\int \frac{\mathbf{J}(\mathbf{r}_2)}{r_{12}} d\tau_2, \quad \mathbf{A}(\mathbf{r}_1) = \frac{\mu_0}{4\pi}\int \frac{\mathbf{K}(\mathbf{r}_2)}{r_{12}} da_2. \tag{8.26}$$

The magnetic vector potential is less useful than the electric scalar potential in electrostatics because the former is still a vector having three components and also because, unlike an electric potential that we can connect to a measurable quantity, there is no direct measure of the vector potential. Introduction of this vector potential nevertheless simplifies the calculations because its integrand contains no cross-product.

Example 8.4 A spherical shell of radius R carries a uniformly distributed surface charge σ. The sphere is spinning at constant angular velocity ω. Find the vector potential $\mathbf{A}$ and magnetic field $\mathbf{B}$ both inside and outside the sphere. This problem resembles that in Griffiths 1999, p. 236, example 5.11.

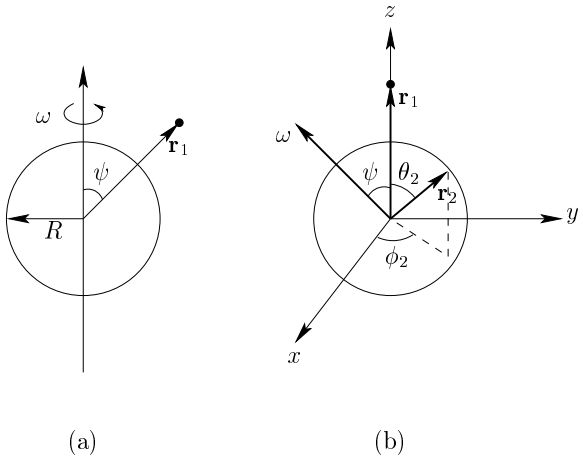


Figure 8.4: A spinning charged sphere.

Solution To solve this problem we use a trick. Although it seems natural to align the z axis along $\boldsymbol{\omega}$, as in Figure 8.4(a), the integral is easier to evaluate if we let $\mathbf{r}_1$ lie on the z axis; then $\boldsymbol{\omega}$ is tilted at an angle ψ on the xz plane: see Figure 8.4(b). We explain the reasoning as follows. Because with such coordinates we have

$$\mathbf{r}_1 = z_1\hat{\mathbf{z}}, \quad \mathbf{r}_2 = R\sin\theta_2\cos\phi_2\hat{\mathbf{x}} + R\sin\theta_2\sin\phi_2\hat{\mathbf{y}} + R\cos\theta_2\hat{\mathbf{z}},$$

then

$$r_{12} = \sqrt{R^2 + z_1^2 - 2Rz_1\cos\theta_2}.$$

This length is familiar as it appears repeatedly in integrals related to Coulomb's law. According to that experience, we choose to perform the integration in the (b) configuration.

The vector for angular velocity is

$$\boldsymbol{\omega} = \omega\sin\psi\,\hat{\mathbf{x}} + \omega\cos\psi\,\hat{\mathbf{z}};$$

hence the velocity $\mathbf{v}_2$ is

$$\begin{aligned}\mathbf{v}_2 &= \boldsymbol{\omega} \times \mathbf{r}_2 \\ &= -R\omega \cos\psi \sin\theta_2 \sin\phi_2 \, \hat{\mathbf{x}} + R\omega(\cos\psi \sin\theta_2 \cos\phi_2 - \sin\psi \cos\theta_2) \, \hat{\mathbf{y}} \\ &\quad + R\omega \sin\psi \sin\theta_2 \sin\phi_2 \, \hat{\mathbf{z}}.\end{aligned}$$

Again, only A_y is nonvanishing because the integrand for A_x and A_z contains $\sin\phi_2$,

$$A_y = \frac{\mu_0}{4\pi} \int_0^{2\pi} d\phi_2 \int_0^{\pi} d\theta_2 \frac{\sigma R\omega(\cos\psi \sin\theta_2 \cos\phi_2 - \sin\psi \cos\theta_2) R^2 \sin\theta_2}{\sqrt{R^2 + z_1^2 - 2Rz_1 \cos\theta_2}}. \quad (8.27)$$

Although this integral appears formidable, Maple achieves the integration and delivers elegant results, depending on whether $\mathbf{r}_1$ is inside or outside the sphere:

$$A_y = \begin{cases} -\dfrac{\mu_0 R\omega\sigma}{3} z_1 \sin\psi, & r \le R, \\ -\dfrac{\mu_0 R^4 \omega\sigma}{3} \dfrac{\sin\psi}{z_2^2}, & r \ge R. \end{cases} \quad (8.28)$$

Worksheet 8.4 Like many preceding worksheets, we define the symbols in a systematic fashion and follow the formulas provided to perform the calculations. The `Norm` command is used as before, and the surface current density `k` is obtained from the `CrossProduct` and `ScalarMultiply` commands. The `int` command serves to evaluate those formidable integrals.

```
> with(LinearAlgebra):
> assume(R>0, theta2, real, phi2, real, z1>0);
> additionally(z1<R); #change to (z1>R) for outside the sphere
> angularvel := < omega*sin(psi) | 0 | omega*cos(psi) >;
```

$$angularvel := [\omega \sin(\psi),\ 0,\ \omega \cos(\psi)]$$

```
> r1vec := < 0 | 0 | z1 >;
```

$$r1vec := [0,\ 0,\ z1]$$

```
> r2vec := < R*sin(theta2)*cos(phi2) | R*sin(theta2)*sin(phi2) |
> R*cos(theta2) >;
```

$$r2vec := [R \sin(\theta 2) \cos(\phi 2),\ R \sin(\theta 2) \sin(\phi 2),\ R \cos(\theta 2)]$$

```
> r12vec := r1vec - r2vec;
```

$$r12vec := [-R \sin(\theta 2) \cos(\phi 2),\ -R \sin(\theta 2) \sin(\phi 2),\ z1 - R \cos(\theta 2)]$$

```
> r12 := Norm(r12vec, 2):  r12 := simplify(r12);
```

$$r12 := \sqrt{R^2 + z1^2 - 2\, z1\, R \cos(\theta 2)}$$

```
> v2 := CrossProduct(angularvel, r2vec);
```

$$v2 := [-\omega \cos(\psi)\, R \sin(\theta 2) \sin(\phi 2),\ \omega \cos(\psi)\, R \sin(\theta 2) \cos(\phi 2) - \omega \sin(\psi)\, R \cos(\theta 2), \omega \sin(\psi)\, R \sin(\theta 2) \sin(\phi 2)]$$

```
> k := ScalarMultiply(v2, sigma);
```

$$k := [-\sigma\,\omega\cos(\psi)\,R\sin(\theta 2)\sin(\phi 2),$$
$$\sigma\,(\omega\cos(\psi)\,R\sin(\theta 2)\cos(\phi 2) - \omega\sin(\psi)\,R\cos(\theta 2)), \sigma\,\omega\sin(\psi)\,R\sin(\theta 2)\sin(\phi 2)]$$

```
> Ay := mu[0]/(4*Pi)*int(int(k[2]*R^2*sin(theta2)/r12,
> phi2=0..2*Pi), theta2=0..Pi);
```

$$Ay := -\frac{1}{3}\,\mu_0\,\omega\sin(\psi)\,R\,\sigma\,z1$$

The vector potential $\mathbf{A}$ in configuration (b) contains only A_y, thus we can transform back to configuration (a) by aligning $\boldsymbol{\omega}$ with $\hat{\mathbf{z}}$ without altering $\mathbf{A}$. To express $\mathbf{A}$ in a spherical basis, we let the position vector for the field point in spherical coordinates be $\mathbf{r}_1 = (r = z_1, \theta = -\psi, \phi = 0)$, and use $\hat{\mathbf{y}} = \hat{\boldsymbol{\phi}}$ in equation (6.18):

$$\mathbf{A}(r,\theta,\phi) = \begin{cases} \dfrac{\mu_0 R\omega\sigma}{3} r\sin\theta\,\hat{\boldsymbol{\phi}}, & r \le R, \\ \dfrac{\mu_0 R^4\omega\sigma}{3}\dfrac{\sin\theta}{r^2}\,\hat{\boldsymbol{\phi}}, & r \ge R. \end{cases} \tag{8.29}$$

The vector potential has the same direction as the current. We calculate the magnetic field by taking the curl of the magnetic vector potential in spherical coordinates:

$$\mathbf{B} = \nabla\times\mathbf{A} = \begin{cases} \dfrac{2}{3}\mu_0 R\omega\sigma\,(\cos\theta\hat{\mathbf{r}} - \sin\theta\hat{\boldsymbol{\theta}}), & r \le R, \\ \dfrac{1}{3}\mu_0 R^4\omega\sigma\,\left(\dfrac{2\cos\theta}{r^3}\hat{\mathbf{r}} + \dfrac{\sin\theta}{r^3}\hat{\boldsymbol{\theta}}\right), & r \ge R. \end{cases} \tag{8.30}$$

Worksheet 8.5 To evaluate the curl of a vector we invoke the `VectorCalculus` package. Because in curvilinear coordinates basis vectors depend on position, we must construct the vector potential $\mathbf{A}$ as a vector field, using the `VectorField` command, so that we can apply `Curl` to it. Special attention is required when we use Maple to plot in spherical coordinates; in some textbooks the definitions of θ and ϕ are interchanged. In Maple, three arguments are required: the first is the radius r, the second is the azimuthal angle ϕ, measured in the xy plane from the x axis, and the third is the angle θ from the z axis. Confusing the order would produce an incorrect graph.

```
> with(LinearAlgebra): with(VectorCalculus): with(plots):

Warning, the names CrossProduct and DotProduct have been rebound

Warning, the assigned names <,> and <|> now have a global binding

Warning, these protected names have been redefined and unprotected: *,
+, ., Vector, diff, int, limit, series

Warning, the name changecoords has been redefined
```

```
> assume(mu[0]>0, R>0, sigma>0, omega>0);
> SetCoordinates( 'spherical'[r, theta, phi]);
```

$$spherical_{r,\theta,\phi}$$

```
> Ain := VectorField(< 0 | 0 | mu[0]*R*omega*sigma/3*r*sin(theta)
> >);
```

$$Ain := \frac{1}{3}\,\mu_0\,R\,\omega\,\sigma\,r\,\sin(\theta)\bar{\mathbf{e}}_{\boldsymbol{\phi}}$$

```
> Aout := VectorField(< 0 | 0 | mu[0]*R^4*omega*sigma/3
> *sin(theta)/r^2 >);
```

$$Aout := \frac{1}{3}\,\frac{\mu_0\,R^4\,\omega\,\sigma\,\sin(\theta)}{r^2}\bar{\mathbf{e}}_{\boldsymbol{\phi}}$$

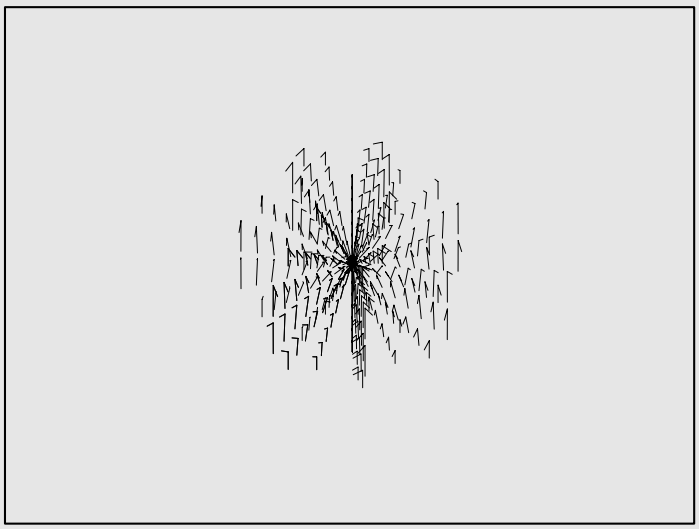
```
> Bin := Curl(Ain, 'spherical'[r, theta, phi]);
```

$$Bin := \frac{2}{3}\,\mu_0\,R\,\omega\,\sigma\,\cos(\theta)\bar{\mathbf{e}}_{\mathbf{r}} - \frac{2}{3}\,\sin(\theta)\,\mu_0\,R\,\omega\,\sigma\bar{\mathbf{e}}_{\boldsymbol{\theta}}$$

```
> Bout := Curl(Aout, 'spherical'[r, theta, phi]);
```

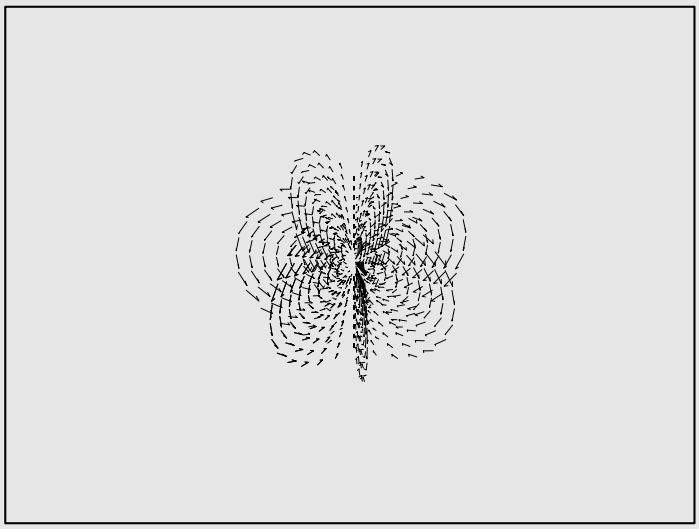
$$Bout := \frac{2}{3}\,\frac{\mu_0\,R^4\,\omega\,\sigma\,\cos(\theta)}{r^3}\bar{\mathbf{e}}_{\mathbf{r}} + \frac{1}{3}\,\frac{\sin(\theta)\,\mu_0\,R^4\,\omega\,\sigma}{r^3}\bar{\mathbf{e}}_{\boldsymbol{\theta}}$$

```
> Binnorm := Normalize(Bin, 2):  Binnorm := map(simplify, Binnorm):
> fieldplot3d([ Binnorm[1], Binnorm[3], Binnorm[2]], r=0..1,
> phi=0..2*Pi, theta=0..Pi, coords=spherical, scaling=constrained);
```



```
> Boutnorm := Normalize(Bout): Boutnorm := map(simplify, Boutnorm):
```

```
> fieldplot3d([ Boutnorm[1], Boutnorm[3], Boutnorm[2]], r=1..5,
> phi=0..2*Pi, theta=0..Pi, coords=spherical, grid=[8,8,16],
> scaling=constrained);
```



The magnetic field inside the sphere is uniform; this fact is readily verifiable from equation (8.30), on transforming from the spherical basis to the Cartesian one, which is $\hat{\mathbf{z}} = \cos\theta\,\hat{\mathbf{r}} - \sin\theta\,\hat{\boldsymbol{\theta}}$ in equation (6.18). Outside the sphere, the pattern of the magnetic field resembles the electric field of an electric dipole discussed in Section 6.5. The dependence on r^{-3} in the magnetic field indicates that a spinning sphere of charge constitutes a magnetic dipole. Explicitly, the magnetic field produced by an ideal (infinitely small) magnetic dipole $\mathbf{m}$ aligned with the z axis at the origin is

$$\mathbf{B} = \frac{\mu_0 m}{4\pi r^3}(2\cos\theta\,\hat{\mathbf{r}} + \sin\theta\,\hat{\boldsymbol{\theta}}). \tag{8.31}$$

Curiously, the electric field produced by an ideal electric dipole $\mathbf{p}$ aligned with the z axis at the origin is

$$\mathbf{E} = \frac{p}{4\pi\epsilon_0 r^3}(2\cos\theta\,\hat{\mathbf{r}} + \sin\theta\,\hat{\boldsymbol{\theta}}). \tag{8.32}$$

Although the electric dipole field is due to charges, and the magnetic dipole field is due to circulating currents, they take the same form. As early as 1821, Ampère suggested that magnetism originates from a "molecular current," and his view was astonishingly prescient because at that time the existence of molecules was not generally accepted. According to modern atomic theory, magnetization of materials indeed arises from circulating currents within atoms, either from intrinsic spin of electrons or from orbital motion of electrons in an atom; see Section 13.5 for details. Our calculation provides a naive model of an electron, which

for this purpose can be considered to be a tiny spinning sphere of charge, such as a magnetic dipole. A neutron, which can also be considered to be a spinning sphere, has a nonvanishing dipole moment anti-parallel to the direction of its angular momentum; this condition indicates that a neutron comprises charged substructures which can be attributed to quarks.

8.4 Force and Torque on Magnetic Dipoles

Because there appears to exist no magnetic monopole, the basic entity in magnetic phenomena involves a magnetic dipole. We devote our attention to the force and torque on magnetic dipoles. All results in this section are applicable to electricity, with replacements $\mathbf{m} \to \mathbf{p}$ and $\mathbf{B} \to \mathbf{E}$. This subject is important in many areas: for example, the dominant force among electrically neutral but electrically polar molecules is due to dipole-dipole interaction.

We have seen two examples for magnetic dipoles: a current loop, and a spinning sphere of charge. A magnetic dipole moment is a vector quantity, of which the direction is normal to the plane of the loop:

$$\mathbf{m} \equiv I \int d\mathbf{a} = I\mathbf{a}. \tag{8.33}$$

We mention in Section 6.5 that an electric dipole consists of two equal but opposite charges a distance apart, but a more general definition for an electric dipole moment is

$$\mathbf{p} \equiv \int \mathbf{r}_2 \, \rho(\mathbf{r}_2) \, d\tau_2. \tag{8.34}$$

A magnetic dipole experiences a torque in a magnetic field:

$$\mathbf{N} = \mathbf{m} \times \mathbf{B}. \tag{8.35}$$

The potential energy depends on the orientation of the dipole in the field:[1]

$$U = -\mathbf{m} \cdot \mathbf{B}, \tag{8.36}$$

and the negative gradient of this potential energy produces a force:

$$\mathbf{F} = \nabla(\mathbf{m} \cdot \mathbf{B}). \tag{8.37}$$

In a uniform field, the net force on a magnetic dipole is zero. For this reason, in the Stern–Gerlach experiment a nonuniform magnetic field is required to separate atoms of differently oriented magnetic dipole moment.[2]

[1] This energy is incomplete in describing a mechanical system, but is sufficient for calculating the force based on the principle of virtual work. We refrain from digressing to a subtlety; see Feynman 1965, vol. 2, p. 15-2ff for details.

[2] An introduction of the Stern–Gerlach experiment can be found in Feynman 1965, vol. 2, p. 35-3ff, and A. P. French and E. F. Taylor, *An Introduction to Quantum Physics*, New York: Norton, 1978, p. 432ff.

The magnetic field produced by an ideal dipole is given in equation (8.31); in coordinate-independent form it appears as

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi r^3}[3(\mathbf{m}\cdot\hat{\mathbf{r}})\hat{\mathbf{r}} - \mathbf{m}], \tag{8.38}$$

where $\hat{\mathbf{r}}$ is the unit vector directed from the dipole to the field point $\mathbf{r}$.

Example 8.5 Find the force and torque between two magnetic dipoles $\mathbf{m}_1$ and $\mathbf{m}_2$ a distance r apart, oriented as shown in Figure 8.5; assume r to be much greater than the physical dimension of the dipoles, so that we can treat the dipoles as ideal.

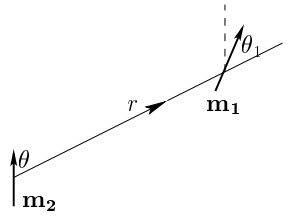


Figure 8.5: Force and torque between two dipoles.

Solution In this example we make use of both Cartesian and spherical coordinates, depending on convenience. Aligning the z axis with $\mathbf{m}_2$, two magnetic dipole moments in the Cartesian basis are

$$\mathbf{m}_2 = m_2\hat{\mathbf{z}}, \quad \mathbf{m}_1 = m_1\sin(\theta-\theta_1)\,\hat{\mathbf{x}} + m_1\cos(\theta-\theta_1)\,\hat{\mathbf{z}}, \tag{8.39}$$

and the position vector is

$$\mathbf{r} = r\sin\theta\,\hat{\mathbf{x}} + r\cos\theta\,\hat{\mathbf{z}}. \tag{8.40}$$

We regard $\mathbf{m}_2$ as the source, and at $\mathbf{r}$ the magnetic field produced by this source is

$$\mathbf{B}_2(\mathbf{r}) = \frac{\mu_0 m_2}{4\pi r^3}\left[3\cos\theta\sin\theta\,\hat{\mathbf{x}} + (3\cos^2\theta - 1)\hat{\mathbf{z}}\right]. \tag{8.41}$$

The potential energy is

$$U = -\mathbf{m}_1\cdot\mathbf{B}_2 = \frac{\mu_0 m_1 m_2}{4\pi r^3}(\sin\theta\sin\theta_1 - 2\cos\theta\cos\theta_1). \tag{8.42}$$

The force is the gradient of $\mathbf{m}_1\cdot\mathbf{B}_2$; we calculate it in spherical coordinates:

$$\mathbf{F} = \nabla(\mathbf{m}_1\cdot\mathbf{B}_2) = \\ \frac{\mu_0 m_1 m_2}{4\pi r^4}[3(\sin\theta\sin\theta_1 - 2\cos\theta\cos\theta_1)\hat{\mathbf{r}} - (\cos\theta\sin\theta_1 + 2\sin\theta\cos\theta_1)\hat{\boldsymbol{\theta}}]. \tag{8.43}$$

The torque is $\mathbf{m}_1\times\mathbf{B}_2$; we calculate it in Cartesian coordinates:

$$\mathbf{N} = \mathbf{m}_1\times\mathbf{B}_2 = \frac{\mu_0 m_1 m_2}{4\pi r^3}(\sin\theta\cos\theta_1 + 2\cos\theta\sin\theta_1)\hat{\mathbf{y}}. \tag{8.44}$$

Worksheet 8.6 The symbols in this worksheet are self-evident. We use spherical coordinates in `Gradient`, although a reader might well use Cartesian coordinates by expressing r and θ in terms of x and z.

```
> assume(r>0, theta, real):
> with(LinearAlgebra): with(VectorCalculus):

Warning, the names CrossProduct and DotProduct have been rebound

Warning, the assigned names <,> and <|> now have a global binding

Warning, these protected names have been redefined and unprotected: *,
+, ., Vector, diff, int, limit, series
> rvec := < r*sin(theta) | 0 | r*cos(theta) >;
```

$$rvec := r\sin(\theta)\,\mathbf{e_x} + r\cos(\theta)\,\mathbf{e_z}$$

```
> m2vec := < 0 | 0 | m2 >;
```

$$m2vec := m2\,\mathbf{e_z}$$

```
> m1vec := < m1*sin(theta-theta1) | 0 | m1*cos(theta-theta1) >;
```

$$m1vec := m1\,\sin(\theta-\theta1)\,\mathbf{e_x} + m1\,\cos(\theta-\theta1)\,\mathbf{e_z}$$

```
> e := Normalize(rvec, 2):
> e := map(simplify, e);
```

$$e := [\sin(\theta),\, 0,\, \cos(\theta)]$$

```
> B2vec := ScalarMultiply((ScalarMultiply(e, 3*DotProduct(m2vec,
e)) - m2vec), mu[0]/(4*Pi*r^3));
```

$$B2vec := \left[\frac{3}{4}\,\frac{\mu_0\,m2\cos(\theta)\sin(\theta)}{\pi\,r^3},\, 0,\, \frac{1}{4}\,\frac{\mu_0\,(3\,m2\cos(\theta)^2 - m2)}{\pi\,r^3}\right]$$

```
> U := -DotProduct(m1vec, B2vec):
> U := combine(U): U := expand(U);
```

$$U := -\frac{1}{2}\,\frac{m1\,\mu_0\,m2\cos(\theta)\cos(\theta1)}{\pi\,r^3} + \frac{1}{4}\,\frac{m1\,\mu_0\,m2\sin(\theta)\sin(\theta1)}{\pi\,r^3}$$

```
> F := -Gradient(U, 'spherical'[r, theta, phi]):
> F := map(simplify, F);
```

$$F := \frac{3}{4}\,\frac{m1\,\mu_0\,m2\,(-2\cos(\theta)\cos(\theta1) + \sin(\theta)\sin(\theta1))}{r^4\,\pi}\,\bar{\mathbf{e}}_{\mathbf{r}} - \frac{1}{4}\,\frac{m1\,\mu_0\,m2\,(2\sin(\theta)\cos(\theta1) + \cos(\theta)\sin(\theta1))}{r^4\,\pi}\,\bar{\mathbf{e}}_{\boldsymbol{\theta}}$$

```
> N := CrossProduct(m1vec, B2vec):
> N := map(combine, N): N := map(expand, N);
```

$$N := \left(\frac{1}{4}\,\frac{m1\,\mu_0\,m2\sin(\theta)\cos(\theta1)}{\pi\,r^3} + \frac{1}{2}\,\frac{m1\,\mu_0\,m2\cos(\theta)\sin(\theta1)}{\pi\,r^3}\right)\,\mathbf{e_y}$$

We leave it to the reader to vary values of θ and θ_1, and to observe the direction of the force and torque. One might even place two bar magnets on a smooth table to perform an experiment. We must notice that the force between dipoles depends on r^{-4}, and on their orientations, θ and θ_1. Therefore, the force is not central (see the definition in Section 4.3) because it contains both radial and tangential components.

8.5 Summary of Electromagnetism in Static Conditions

A charged particle is influenced by electric and magnetic forces. Classical electromagnetism is a field theory, in which force represents the interaction between fields and charge according to the Lorentz force law,

$$\mathbf{F} = q[\mathbf{E} + (\mathbf{v} \times \mathbf{B})]. \tag{8.45}$$

Because we can extract measurable physical quantities, such as force, energy and momentum, from fields, the objective is to determine electric and magnetic fields in the region of interest from charge and current according to given distributions, or from boundary conditions. In static conditions, the fields are governed by these four Maxwell's equations:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \tag{8.46a}$$

$$\nabla \times \mathbf{E} = 0, \tag{8.46b}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{8.46c}$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J}. \tag{8.46d}$$

For electric charge and current according to given distributions, the electric field and the magnetic field are calculated by these integrals:

$$\mathbf{E}(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}_2)}{r_{12}^2} \, \mathbf{e}_{12} \, d\tau_2, \tag{8.47}$$

$$\mathbf{B}(\mathbf{r}_1) = \frac{\mu_0}{4\pi} I \int \frac{d\mathbf{l}_2 \times \mathbf{e}_{12}}{r_{12}^2}. \tag{8.48}$$

We consider these two equations to constitute solutions of Maxwell's equations. In principle, we can enter them in Maple, and obtain the results analytically or numerically. Several examples appear in Sections 6.1, 6.2, and 8.2. The most important aspect of the calculation is to distinguish the position vectors for the *source* and the *field*, and their *separation*.

We introduce the electric scalar potential V and the magnetic vector potential $\mathbf{A}$; because they simplify calculations, they may be considered as an intermediate step. Potentials can be evaluated for a given distribution, and once they are determined we calculate the fields:

$$V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}_2)}{r_{12}} d\tau_2, \quad \mathbf{E} = -\nabla V, \tag{8.49}$$

and

$$\mathbf{A}(\mathbf{r}_1) = \frac{\mu_0}{4\pi} I \int \frac{d\mathbf{l}_2}{r_{12}}, \quad \mathbf{B} = \nabla \times \mathbf{A}. \tag{8.50}$$

We offer examples in Section 6.4 and Section 8.3.

We devote Chapter 7 to the theory of potential, which provides an extremely useful technique for obtaining the electric potential from boundary conditions. We neglect the application of the symmetry properties of Gauss's law and Ampère's law; problems of this type can certainly be solved with Maple, but in most situations manual calculation is easy.

Exercises

1. Find the trajectory of a charged particle when both uniform electric and magnetic fields are present, the same as for the example in Section 8.1, with the following initial velocities:
   (a) $\mathbf{v}(0) = -(E/B)\,\hat{\mathbf{y}}$;
   (b) $\mathbf{v}(0) = (E/2B)\,\hat{\mathbf{y}}$;
   (c) $\mathbf{v}(0) = (E/B)\,(\hat{\mathbf{y}} + \hat{\mathbf{z}})$.

2. We calculate the magnetic field at a distance z above the center of a circular loop carrying a steady current; that is equation (8.18). Plot the magnetic field as a function of z.

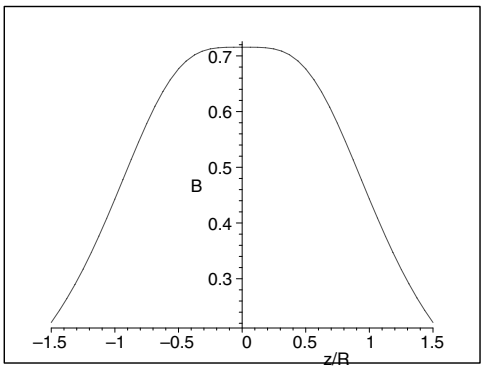


Figure 8.6: The Helmholtz coil provides a convenient way of producing a relatively uniform magnetic field near its center.

3. The Helmholtz coil comprises two current loops of radius R a distance d apart. (a) Find the expression for the magnetic field on the axis as a function of z, and show that $\partial B/\partial z$ is zero at the midway point. (b) Determine d such that $\partial^2 B/\partial z^2$ is also zero at the midpoint (*Answer*: $d = R$), and calculate the resulting magnetic field there. (c) Plot the magnetic field as a function of z for such d, which should resemble Figure 8.6.

4. A semicircular wire carries a steady current i; see Figure 8.7. Find the magnetic field at a point P on the other semicircle. This problem is taken from Griffiths 1999, p. 249, problem 5.45.

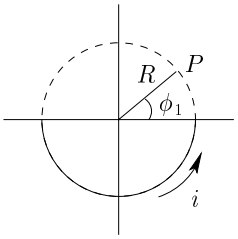


Figure 8.7: Semicircular wire carrying a current.

5. Two straight conductors of infinite length are placed parallel to the z axis, a distance d apart and each carries current i in opposite directions. Determine the vector potential of this system.

6. A uniformly charged sphere of radius R carries a total charge q; the sphere is rotated about a diameter with constant angular velocity ω. Calculate the vector potential and magnetic field both inside and outside the sphere.

7. This exercise guides the reader to calculate the magnetic field produced by a circular loop of radius R lying in the xy plane and carrying a current i using multipole expansion.[3] For a field point on the xz plane (see Figure 8.8), we use equation (6.46) to expand the separation vector:

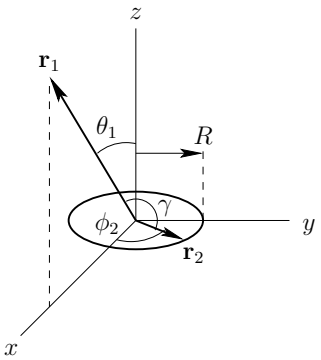


Figure 8.8: Circular wire carrying a current.

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \frac{R^l}{r_1^{l+1}} P_l(\cos\gamma), \quad \text{for } r_1 > R, \tag{8.51}$$

[3] One might consult Jackson 1999, p. 184, equations (5.46), (5.48), (5.49).

where

$$\cos\gamma = \sin\theta_1 \cos\phi_2;$$

this expression is from equation (6.45b) with $\phi_1 = 0$ and $\theta_2 = \pi/2$.

(a) From equation (8.25), we write

$$\begin{aligned} A_y = \frac{\mu_0}{4\pi} i \Bigg[& \frac{1}{r_1} \int_0^{2\pi} P_0(\cos\gamma) R\cos\phi_2 d\phi_2 \\ & + \frac{1}{r_1^2} \int_0^{2\pi} R P_1(\cos\gamma) R\cos\phi_2 d\phi_2 \\ & + \frac{1}{r_1^3} \int_0^{2\pi} R^2 P_2(\cos\gamma) R\cos\phi_2 d\phi_2 \\ & + \frac{1}{r_1^4} \int_0^{2\pi} R^3 P_3(\cos\gamma) R\cos\phi_2 d\phi_2 + \ldots \Bigg]. \end{aligned} \tag{8.52}$$

Evaluate these integrals (P_l can be invoked with the `LegendreP` command) to verify that

$$A_y = \frac{\mu_0}{4\pi} i\pi R^2 \left[\frac{1}{r_1^2} \sin\theta_1 - \frac{R^2}{4r_1^4} P_{31}(\cos\theta_1) + \frac{R^4}{8r_1^6} P_{51}(\cos\theta_1) + \ldots \right], \tag{8.53}$$

where

$$P_{31}(\cos\theta) = \frac{15}{2}\sin\theta\cos^2\theta - \frac{3}{2}\sin\theta,$$

$$P_{51}(\cos\theta) = \frac{315}{8}\sin\theta\cos^4\theta - \frac{105}{4}\sin\theta\cos^2\theta + \frac{15}{8}\sin\theta.$$

These P_{lm} are the associated Legendre polynomials. One need not be concerned with the names; we will discuss them in Section 16.2, equation (16.11).

(b) In spherical coordinates, the vector potential is

$$\mathbf{A} = A_\phi \hat{\boldsymbol{\phi}},$$

where $A_\phi = A_y$ as obtained in equation (8.53). Use Maple's `Curl` command to verify that the magnetic field is

$$\begin{aligned} \mathbf{B} = \frac{\mu_0}{4\pi} i\pi R^2 \Bigg\{ & 2\left[\frac{1}{r_1^3}\cos\theta_1 - \frac{3R^2}{2r_1^5} P_3(\cos\theta_1) + \frac{15R^4}{8r_1^5} P_5(\cos\theta_1) + \ldots \right] \hat{\mathbf{r}} \\ & + \left[\frac{1}{r_1^3}\sin\theta_1 - \frac{3R^2}{4r_1^5} P_{31}(\cos\theta_1) + \frac{5R^4}{8r_1^5} P_{51}(\cos\theta_1) + \ldots \right] \hat{\boldsymbol{\theta}} \Bigg\}, \end{aligned} \tag{8.54}$$

where the Legendre polynomials are

$$P_3(\cos\theta) = \frac{5}{2}\cos^3\theta - \frac{3}{2}\cos\theta,$$

$$P_5(\cos\theta) = \frac{63}{8}\cos^5\theta - \frac{35}{4}\cos^3\theta + \frac{15}{8}\cos\theta.$$

8. A physical electric dipole consists of two equal and opposite charges separated by a distance d; see Figure 8.9.

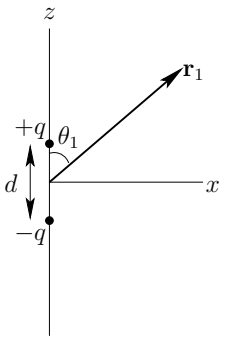


Figure 8.9: Physical electric dipole.

(a) Verify that the electric potential of this system is

$$V = \frac{1}{4\pi\epsilon_0}qd\left[\frac{1}{r_1^2}\cos\theta + \frac{d^2}{4r_1^4}P_3(\cos\theta_1) + \frac{d^4}{16r_1^6}P_5(\cos\theta_1) + \ldots\right]. \quad (8.55)$$

This problem actually belongs to Chapter 6; one might review the discussion of multipole expansion in Section 6.4.2.

(b) Use Maple's `Gradient` command in spherical coordinates to verify that the electric field is

$$\mathbf{E} = \frac{1}{4\pi\epsilon_0}qd\left\{2\left[\frac{1}{r_1^3}\cos\theta_1 + \frac{d^2}{2r_1^5}P_3(\cos\theta_1) + \frac{3d^4}{16r_1^7}P_5(\cos\theta_1) + \ldots\right]\hat{\mathbf{r}}\right.$$
$$\left. + \left[\frac{1}{r_1^3}\sin\theta_1 + \frac{d^2}{4r_1^5}P_{31}(\cos\theta_1) + \frac{d^4}{16r_1^7}P_{51}(\cos\theta_1) + \ldots\right]\hat{\boldsymbol{\theta}}\right\}. \quad (8.56)$$

(c) Comparing equations (8.54) and (8.56), comment on the similarity and difference between electric and magnetic dipoles.

9. Using equation (8.1), the Lorentz force law, and equations (8.31) and (8.32), consider the motion of an electric charge in magnetic and electric dipole fields.[4]

[4]See G. C. McGuire, "Using computer algebra to investigate the motion of an electric charge in magnetic and electric dipole fields," *American Journal of Physics*, **71**, 809–812 (2003).

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9 Electric Circuits

Many problems of simple electric circuits involve solving a system of equations simultaneously; as we have seen in Chapter 1, Maple is particularly suitable for this type of problem. The mathematical structure of an oscillatory circuit is identical to that of a spring-mass system in mechanics, treated in Chapter 2, for which we solve second-order linear differential equations. Alternating circuits have the same mathematical structure as forced oscillations, but in this chapter we introduce a technique of using complex numbers to solve the problems.

9.1 Resistors in Series and in Parallel

Ohm's law is

$$V = IR. \tag{9.1}$$

The resistance of resistors connected in series is the sum of their individual resistances,

$$R = R_1 + R_2 + R_3 + \ldots. \tag{9.2}$$

The resistance of resistors connected in parallel is

$$\frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2} + \frac{1}{R_3} + \ldots. \tag{9.3}$$

One can analyze a complicated circuit by repeatedly combining elements using the above formulas to reduce it to a simple circuit. We offer two examples.

Example 9.1 Derive the formula for the delta-star (or Δ-Y) transformation.

Solution From Figure 9.1, we find R_a, R_b and R_c by solving these equations:

$$R_a + R_b = \frac{1}{\frac{1}{R_1} + \frac{1}{R_2+R_3}}, \tag{9.4a}$$

$$R_a + R_c = \frac{1}{\frac{1}{R_2} + \frac{1}{R_1+R_3}}, \tag{9.4b}$$

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ISBN: 3-527-40640-9

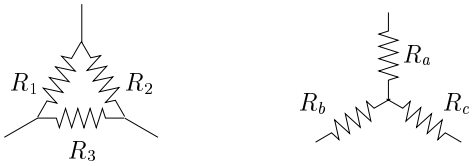


Figure 9.1: Δ-Y transformation.

and

$$R_b + R_c = \frac{1}{\frac{1}{R_3} + \frac{1}{R_1+R_2}}. \tag{9.4c}$$

We obtain

$$R_a = \frac{R_1 R_2}{R_1 + R_2 + R_3}, \quad R_b = \frac{R_1 R_3}{R_1 + R_2 + R_3}, \quad R_c = \frac{R_2 R_3}{R_1 + R_2 + R_3}. \tag{9.5}$$

Worksheet 9.1 We have three equations and three unknowns. We denote `Ra` as R_a, `R1` as R_1 etc., and use the `solve` command to evaluate the unknowns.

```
> Eq1 := Ra + Rb = 1/(1/R1 + 1/(R2+R3));
```

$$Eq1 := Ra + Rb = \frac{1}{\frac{1}{R1} + \frac{1}{R2 + R3}}$$

```
> Eq2 := Ra + Rc = 1/(1/R2 + 1/(R1+R3));
```

$$Eq2 := Ra + Rc = \frac{1}{\frac{1}{R2} + \frac{1}{R1 + R3}}$$

```
> Eq3 := Rb + Rc = 1/(1/R3 + 1/(R1+R2));
```

$$Eq3 := Rb + Rc = \frac{1}{\frac{1}{R3} + \frac{1}{R1 + R2}}$$

```
> solve({Eq1, Eq2, Eq3}, {Ra, Rb, Rc});
```

$$\left\{ Rc = \frac{R2\ R3}{R2 + R3 + R1},\ Rb = \frac{R1\ R3}{R2 + R3 + R1},\ Ra = \frac{R1\ R2}{R2 + R3 + R1} \right\}$$

Example 9.2 The value of an unknown resistance can be accurately measured with a circuit known as the Wheatstone bridge, shown in Figure 9.2. The circuit consists of unknown resistor R_x, three known resistors R_1, R_2, R_3, and a galvanometer; the resistance of the known resistor R_1 is varied until the galvanometer reading is zero. Derive the balance condition.

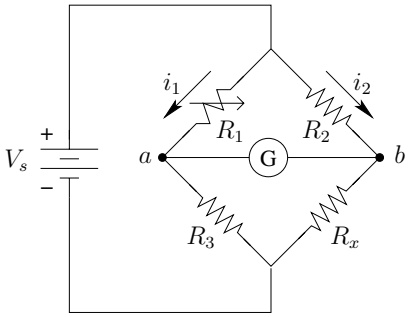


Figure 9.2: Wheatstone bridge.

Solution If there is no current between a and b, we can set two equations:

$$i_1(R_1 + R_3) = i_2(R_2 + R_x),$$

$$i_1 R_1 = i_2 R_2.$$

Having three unknowns, i_1, i_2 and R_x, but only two equations, we can solve for the ratio. Doing so we obtain

$$R_x = \frac{R_2 R_3}{R_1}. \tag{9.6}$$

Worksheet 9.2 In this worksheet, the corresponding symbols are evident. For three unknowns, `Rx`, `i1` and `i2`, we only have two equations. We choose a subset of unknowns `Rx` and `i2` and ask Maple to return the solutions in terms of another unknown `i1`. Avoid using the symbol `I` that Maple reserves for the imaginary unit, $\sqrt{-1}$.

```
> Eq1 := i1*R1 + i1*R3 = i2*R2 + i2*Rx;
```

$$Eq1 := i1\ R1 + i1\ R3 = i2\ R2 + i2\ Rx$$

```
> Eq2 := i1*R1 = i2*R2;
```

$$Eq2 := i1\ R1 = i2\ R2$$

```
> Soln1 := solve({Eq1, Eq2}, {Rx, i2});
```

$$Soln1 := \left\{ i2 = \frac{i1\ R1}{R2},\ Rx = \frac{R3\ R2}{R1} \right\}$$

9.2 Kirchhoff's Rules

Although a complicated circuit may be analyzed by reducing series and parallel components to their equivalents, there exist simple circuits for which analysis according to this method fails.

Kirchhoff's rules are applicable to any circuit; they are based on two fundamental theorems in electromagnetism: electric charge is conserved, and the curl of electric field is zero in electrostatic conditions. The latter,

$$\nabla \times \mathbf{E} = 0,$$

is one of Maxwell's equations. This equation, written in an integral form, signifies that a line integral of electric field around any complete loop is zero,

$$\oint \mathbf{E} \cdot d\mathbf{l} = 0. \tag{9.7}$$

We state Kirchhoff's rules in terms of current and voltage:

1. The sum of currents entering a junction in a circuit equals the sum of currents leaving that junction,

$$\sum I_{\text{in}} = \sum I_{\text{out}}. \tag{9.8}$$

2. The sum of potential differences across all elements around any closed circuit loop is zero,

$$\sum_{\text{closed loop}} \Delta V = 0. \tag{9.9}$$

Example 9.3 In the circuit shown in Figure 9.3, determine the current in each resistor.

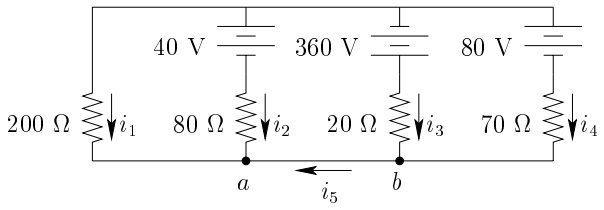


Figure 9.3: A circuit with resistors and batteries.

Solution We adopt labels for currents according to the figure. Applying rule 1, we find at junction a,

$$i_1 + i_2 + i_5 = 0,$$

and at junction b,

$$i_3 + i_4 - i_5 = 0.$$

Applying rule 2, we take the direction of loops to be counterclockwise.

For the left loop,

$$+40 - 200i_1 + 80i_2 = 0;$$

for the middle loop,

$$-360 - 40 - 80i_2 + 20i_3 = 0,$$

and for the right loop,

$$+80 + 360 - 20i_3 + 70i_4 = 0.$$

Solving these five equations simultaneously, we obtain

$$i_1 = -1, \quad i_2 = -3, \quad i_3 = 8, \quad i_4 = -4, \quad i_5 = 4.$$

All magnitudes of current are in units of amperes. A negative current signifies that it flows in the opposite direction to that in which we assign in the diagram.

Worksheet 9.3 In this problem we have five equations for five unknowns. The significance of symbols is obvious.

```
> Eq1 := i1 + i2 + i5 = 0;
```

$$Eq1 := i1 + i2 + i5 = 0$$

```
> Eq2 := i3 + i4 - i5 = 0;
```

$$Eq2 := i3 + i4 - i5 = 0$$

```
> Eq3 := 40 - 200*i1 + 80*i2 = 0;
```

$$Eq3 := 40 - 200\,i1 + 80\,i2 = 0$$

```
> Eq4 := -360 - 40 - 80*i2 + 20*i3 = 0;
```

$$Eq4 := -400 - 80\,i2 + 20\,i3 = 0$$

```
> Eq5 := 80 + 360 - 20*i3 + 70*i4 = 0;
```

$$Eq5 := 440 - 20\,i3 + 70\,i4 = 0$$

```
> Soln1 := solve({Eq1, Eq2, Eq3, Eq4, Eq5}, {i1, i2, i3, i4, i5});
```

$$Soln1 := \{i1 = -1,\ i4 = -4,\ i3 = 8,\ i5 = 4,\ i2 = -3\}$$

9.3 Direct-current Circuits

In addition to resistors, capacitors and inductors are common elements in circuits. Here we discuss direct-current circuits containing these elements.

9.3.1 RC Circuit

Simple RC circuits are shown in Figure 9.4; (a) is a charging circuit, and (b) is a discharging circuit.

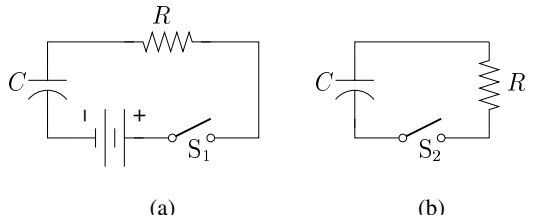


Figure 9.4: Simple RC circuits.

We discuss the RC charging circuit. According to Kirchhoff's rule and supposing the battery to have voltage V_0, after closing switch S_1, we write for a counterclockwise loop starting at the battery,

$$V_0 - iR - \frac{q}{C} = 0. \tag{9.10}$$

In this equation, q/C is the potential difference across the capacitor, and iR is the potential difference across the resistor. The definition of current is

$$i = \frac{dq}{dt}. \tag{9.11}$$

We rewrite equation (9.10) as

$$V_0 - \frac{dq}{dt}R - \frac{q}{C} = 0. \tag{9.10$'$}$$

The problem of a simple RC circuit thus amounts to simply solving a first-order differential equation, which Maple can readily accomplish. Suppose the capacitor to have no charge at time $t = 0$, so $q(0) = 0$; the solution is

$$q = CV_0\left(1 - e^{-t/RC}\right). \tag{9.12}$$

We also find the current by differentiating charge with respect to time,

$$i = \frac{dq}{dt} = \frac{V_0}{R}e^{-t/RC}. \tag{9.13}$$

This solution indicates an exponential decay of the current as the capacitor charges, according to which we identify the characteristic time constant to be RC.

Worksheet 9.4

```
> Eq1 := V0 - q(t)/C - diff(q(t),t)*R = 0;
```

$$Eq1 := V0 - \frac{\mathrm{q}(t)}{C} - \left(\frac{d}{dt}\,\mathrm{q}(t)\right) R = 0$$

```
> Soln1 := dsolve({Eq1, q(0)=0}, q(t));
```

$$Soln1 := \mathrm{q}(t) = V0\,C - e^{\left(-\frac{t}{C\,R}\right)}\,V0\,C$$

```
> assign(Soln1);
> current := diff(q(t), t);
```

$$current := \frac{e^{\left(-\frac{t}{C\,R}\right)}\,V0}{R}$$

We leave the discharging RC circuit as an exercise.

9.3.2 *RL* Circuit

A simple RL circuit is shown in Figure 9.5.

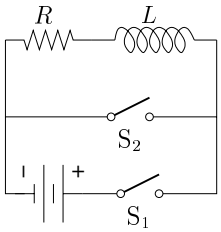


Figure 9.5: Simple RL circuit.

We discuss the situation in which we close S_1 at $t = 0$ while keeping S_2 open. Applying Kirchhoff's rule and proceeding counterclockwise starting from the battery, because the voltage difference across an inductor is $L\frac{di}{dt}$, we obtain

$$V_0 - L\frac{di}{dt} - iR = 0, \tag{9.14}$$

which is also a first-order differential equation. Suppose that there is no initial current at $t = 0$, so that $i(0) = 0$, we solve this equation:

$$i = \frac{V_0}{R}\left(1 - e^{-Rt/L}\right). \tag{9.15}$$

The solution has the form of an exponential decay, in which the characteristic time constant is L/R. The current asymptotically approaches V_0/R, which implies that L ceases to play a role in this circuit after a sufficiently long time.

Worksheet 9.5

```
> Eq1 := V0 - L*diff(i(t),t) = i(t)*R;
```

$$Eq1 := V0 - L\left(\frac{d}{dt}\,\mathrm{i}(t)\right) = \mathrm{i}(t)\,R$$

```
> Soln1 := dsolve({Eq1, i(0)=0}, i(t));
```

$$Soln1 := \mathrm{i}(t) = \frac{V0}{R} - \frac{e^{\left(-\frac{R\,t}{L}\right)}\,V0}{R}$$

9.3.3 *RLC* Circuit

A RLC circuit in series is depicted in Figure 9.6.

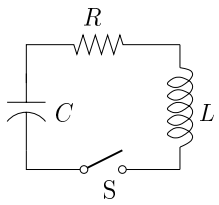


Figure 9.6: Basic RLC circuit in series.

Applying Kirchhoff's rule, clockwise starting from the capacitor, we obtain

$$-\frac{q}{C} - iR - L\frac{di}{dt} = 0. \tag{9.16}$$

With this definition of current,

$$i = \frac{dq}{dt},$$

we rewrite the equation as

$$L\frac{d^2q}{dt^2} + R\frac{dq}{dt} + \frac{q}{C} = 0. \tag{9.17}$$

This equation is identical to the second-order differential equation governing damped oscillation for the spring-mass system,

$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + kx = 0. \tag{9.18}$$

We have studied this type of problem extensively in Chapter 2; all the results obtained there are directly applicable here: we simply need to alter the symbols. We make a list in Table 9.1.

Table 9.1: Mechanical and electric system.

Mechanical system	Electrical system
time, t	time, t
position, x	charge, q
mass, m	inductance, L
damping coefficient, b	resistance, R
spring constant, k	(capacitance)$^{-1}$, 1/C
force, F	voltage, V

Similar to the patterns for damped mechanical oscillation, we classify the solution of differential equations as follows:

1. overdamping, $R^2 > 4L/C$;
2. underdamping, $R^2 < 4L/C$;
3. critical damping, $R^2 = 4L/C$.

Example 9.4 In a typical experiment, we drive an electric circuit with a signal generator and observe the response with an oscilloscope. For the RLC circuit in Figure 9.6, suppose that $R = 50\ \Omega$, $L = 10$ mH and $C = 0.19$ μF. The function generator is operated to output a square wave at electric potential difference 10 V and frequency 300 Hz.

Solution We slightly modify the differential equation to conform to an experimental situation. The function generator outputs 5 V for an interval $1/300$ s, then -5 V for another interval $1/300$ s, and so on. The capacitor is typically fully charged from a previous cycle; therefore, if we choose zero time as the beginning of one cycle, the initial conditions become

$$q(0) = C\,\Delta V = (0.19 \times 10^{-6})(5) = 9.5 \times 10^{-7}\ \text{C},$$

and

$$\dot{q}(0) = 0.$$

The differential equation is

$$L\frac{d^2q}{dt^2} + R\frac{dq}{dt} + \frac{q}{C} = -V_0;$$

note an offset $-V_0$. For the next cycle, because the capacitor is negatively charged, we have the initial conditions

$$q(1/300) = -9.5 \times 10^{7}\ (\text{C}),$$

and

$$\dot{q}(1/300) = 0.$$

The differential equation becomes

$$L\frac{d^2q}{dt^2} + R\frac{dq}{dt} + \frac{q}{C} = V_0.$$

Note the switching of sign of the offset, V_0.

Worksheet 9.6 We solve the differential equations for three cycles, and produce a plot similar to one that would appear on an oscilloscope.

```
> V0:=5; P:=1/300; C:=0.19e-6; R:=50; L:=10e-3;
```

$$V0 := 5$$
$$P := \frac{1}{300}$$
$$C := 0.19\,10^{-6}$$
$$R := 50$$
$$L := 0.010$$

```
> Eq1 := Q1(t)/C + diff(Q1(t),t)*R + L*diff(Q1(t),t$2) = -V0;
```

$$Eq1 := 0.5263157895\,10^{7}\,\mathrm{Q1}(t) + 50\,(\tfrac{d}{dt}\,\mathrm{Q1}(t)) + 0.010\,(\tfrac{d^2}{dt^2}\,\mathrm{Q1}(t)) = -5$$

```
> Soln1 := dsolve({Eq1, Q1(0)=C*V0, D(Q1)(0)=0}, Q1(t));
```

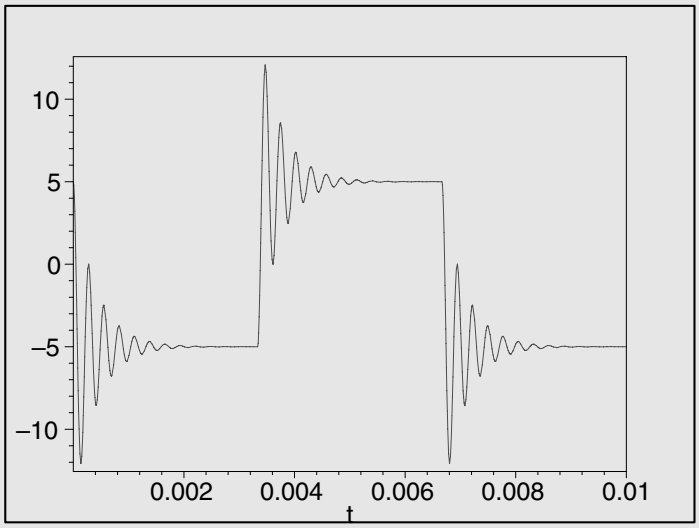
$$Soln1 := \mathrm{Q1}(t)$$
$$= \frac{40000000001}{8759002770964265928000}\,e^{(-2500\,t)}\sin\left(\frac{\sqrt{2080263158}\,t}{2}\right)\sqrt{2080263158}$$
$$+\frac{40000000001}{21052631580000000}\,e^{(-2500\,t)}\cos\left(\frac{\sqrt{2080263158}\,t}{2}\right) - \frac{1000}{1052631579}$$

```
> assign(Soln1);
> Eq2 := Q2(t)/C + diff(Q2(t),t)*R + L*diff(Q2(t),t$2) = V0:
> Soln2 := dsolve({Eq2, Q2(P)=-C*V0, D(Q2)(P)=0}, Q2(t)):
> assign(Soln2):
> Eq3 := Q3(t)/C + diff(Q3(t),t)*R + L*diff(Q3(t),t$2) = -V0:
> Soln3 := dsolve({Eq3, Q3(2*P)=C*V0, D(Q3)(2*P)=0}, Q3(t)):
> assign(Soln3):
> with(plots):

Warning, the name changecoords has been redefined

> p1 := plot(Q1(t)/C, t=0..P):
> p2 := plot(Q2(t)/C, t=P..2*P):
> p3 := plot(Q3(t)/C, t=2*P..3*P):
```

```
> display([p1,p2,p3], axes=BOXED);
```



This pattern is similar to mechanical oscillation in an underdamped condition. We further illustrate a simple application of Maple's graphic ability in a physics laboratory.

9.3.4 Lissajous Figures

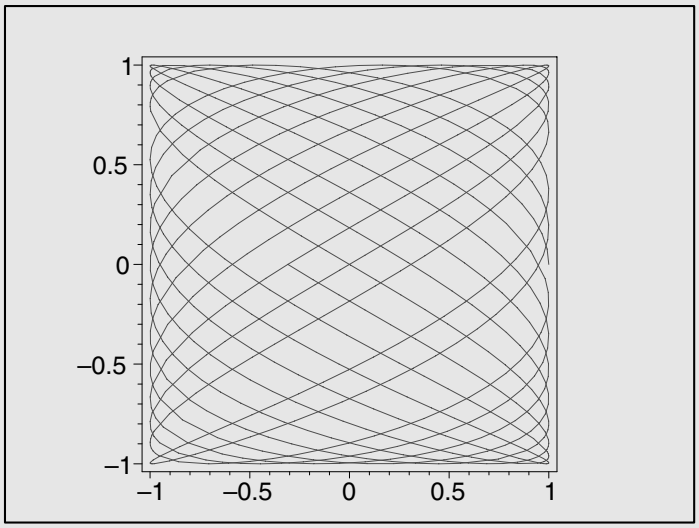
An oscilloscope is an indispensable instrument in a laboratory: it displays voltage as a function of time t, thus allowing experimental verification of a calculated result, as illustrated in the preceding worksheet. In addition to the x–t mode, it is possible to display one voltage against another voltage, or the x–y mode. When two signals are connected to the horizontal and vertical inputs of an oscilloscope, it plots the value of one signal against the value of the other as both signals vary with time. Such a plot is called the Lissajous figure, and from it one can obtain information about phase and amplitude. A parametric plot in Maple simulates such a display on an oscilloscope. We use the following worksheet to illustrate parametric plots.

Worksheet 9.7 To make a parametric plot, one specifies both x and y as functions of some parameter, in this case time t. The syntax to specify a parametric plot is a list (enclosed within square brackets) containing an x expression, a y expression, and the name and range of the parameter.

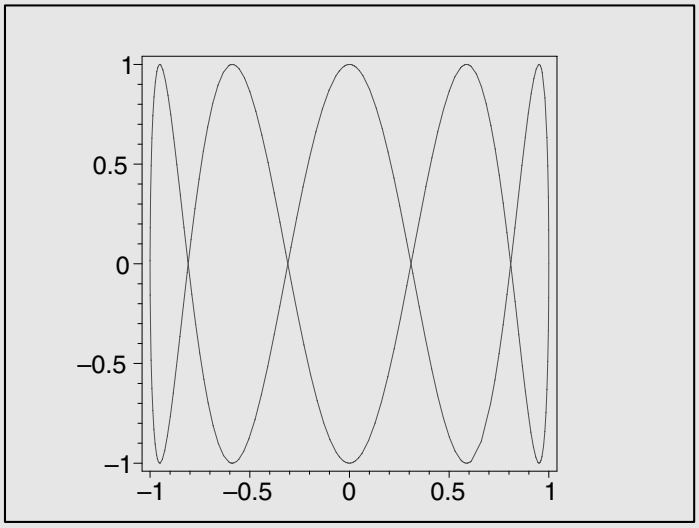
```
> f := 60; omega := 2*Pi*f;
```

$$f := 60$$
$$\omega := 120\,\pi$$

```
> plot([cos(5.1*omega*t), sin(3*omega*t), t=0..3/f],
scaling=constrained, axes=boxed);
```




```
> plot([cos(omega*t), sin(5*omega*t), t=0..1/f],
scaling=constrained, axes=boxed);
```



A reader with experience of operating an oscilloscope might instantly recognize these plots; these Lissajous figures illustrate two ratios of horizontal and vertical frequencies, $5.1 : 3$ and $1 : 5$.

9.4 Alternating-current Circuits

The mathematical structure of a direct-current RLC circuit is identical to that of damped oscillation in mechanics, and an alternating-current circuit corresponds to driven oscillation. We merely need to substitute the symbols in Table 9.1, with the driving force replaced by the voltage. We have demonstrated how to solve this type of differential equation with the `dsolve` command in Chapter 2. In this section, we refrain from repeating the treatment of second-order differential equations; instead we introduce the method with complex numbers to find the steady-state solution. Conversely, this technique is applicable to a mechanical system.

9.4.1 Impedance

For a circuit driven by a sinusoidal voltage, when the system reaches a stable state, the current in an inductor lags behind the voltage across that inductor by $\pi/2$, and the current in a capacitor leads the voltage across that capacitor by $\pi/2$. Across a resistor there is no phase difference. These results can be incorporated into the formulation with complex numbers. In the Cartesian form, a complex number is written as $x + iy$, where x and y are real and $i = \sqrt{-1}$. We can convert the Cartesian form to the polar form,

$$\tilde{\rho} = x + iy = \rho e^{i\varphi}, \quad \left(\rho = \sqrt{x^2 + y^2}, \quad \varphi = \arctan\frac{y}{x}\right).$$

In our notation, a symbol with a tilde is a complex number, and its counterpart without a tilde is its magnitude,

$$\rho = |\tilde{\rho}|.$$

As a complex number intrinsically contains information about magnitude and phase, it provides a convenient representation of an electric circuit in which voltage and current might not oscillate in phase. We offer no derivation of the use of complex numbers in the analysis of an alternating-current circuit, which can be found in much literature,[1] but simply state the rules.

Ohm's law is generalized to

$$\tilde{V} = \tilde{I}\tilde{Z}, \tag{9.19}$$

where $\tilde{V}$, $\tilde{I}$, $\tilde{Z}$ are complex numbers; $\tilde{Z}$ is called the impedance. We make the effort to attach a tilde to a symbol that is a complex number; in some literature these tildes are omitted.

According to this formulation we express complex voltage and current in the polar form,

$$\tilde{V} = Ve^{i\alpha_V}, \quad \tilde{I} = Ie^{i\alpha_I},$$

[1] Feynman 1965, vol. 2, Chapter 22.

where V and I are magnitudes, which are maximum values of voltage and current respectively; α_V and α_I are corresponding phase angles. Do not confuse the imaginary unit $i = \sqrt{-1}$ with current the I.

For a resistor,

$$\tilde{Z}(\text{resistor}) = R, \tag{9.20}$$

which yields Ohm's original law.

For an inductor, the impedance is

$$\tilde{Z}(\text{inductor}) = i\omega L. \tag{9.21}$$

We understand that a rapidly varying field in an inductor enhances the potential; therefore Z is proportional to ω. The property that the current lags behind the voltage by $\pi/2$ in an inductor is reflected in the imaginary factor, because $e^{i\pi/2} = i$.

For a capacitor,

$$\tilde{Z}(\text{capacitor}) = \frac{1}{i\omega C}. \tag{9.22}$$

In this situation, a slowly varying field provides a sufficient time for the capacitor to be charged and hence for the potential to increase; therefore Z is inversely proportional to ω. The property that current leads the voltage by $\pi/2$ is likewise reflected in the imaginary factor, because $e^{-i\pi/2} = -i = 1/i$.

We summarize the impedance in Figure 9.7.

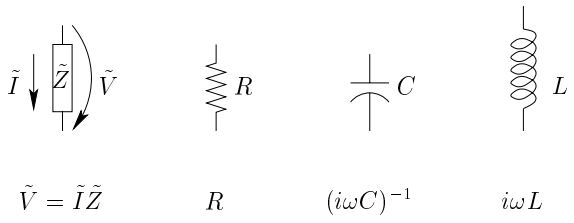


Figure 9.7: Impedance of basic circuit elements.

We can combine impedances to evaluate their equivalent. For a series connection,

$$\tilde{Z} = \tilde{Z}_1 + \tilde{Z}_2 + \tilde{Z}_3 + \ldots, \tag{9.23}$$

and for a parallel connection,

$$\frac{1}{\tilde{Z}} = \frac{1}{\tilde{Z}_1} + \frac{1}{\tilde{Z}_2} + \frac{1}{\tilde{Z}_3} + \ldots. \tag{9.24}$$

We typically control the voltage, and the current is

$$\tilde{I} = \frac{\tilde{V}}{\tilde{Z}}.$$

Any physical quantity is measured by a real number. Once we obtain $\tilde{I}$, we must evaluate its magnitude I and phase angle α_I.

For an alternating current, the magnitude of the voltage $V = |\tilde{V}|$ or the current $I = |\tilde{I}|$ is the maximum value of the oscillation. Customarily, one actually measures the root-mean-square value:

$$V_{\text{rms}} = \frac{V}{\sqrt{2}}, \quad I_{\text{rms}} = \frac{I}{\sqrt{2}}. \tag{9.25}$$

A factor $\sqrt{1/2}$ arises from averaging $\cos^2(\omega t)$ over one cycle, which gives $1/2$.

The average power is

$$\overline{P} = \frac{V_{\text{rms}}^2}{\Re\{\tilde{Z}\}} = I_{\text{rms}}^2 \Re\{\tilde{Z}\}, \tag{9.26}$$

because only the real part dissipates energy. The notation $\Re\{\tilde{Z}\}$ signifies the real part of the impedance $\tilde{Z}$.

Similar to a direct-current circuit, we can reduce elements in series and parallel connection to their equivalent impedance. For a circuit that defies such reduction, we can always apply Kirchhoff's rules.

Example 9.5 An RLC series circuit is driven by a sinusoidal power supply of maximum voltage V at angular frequency ω. (a) Find the maximum current delivered by the source and the phase angle between current and voltage. (b) Calculate the maximum charge in the capacitor.

Solution For RLC in series,

$$\tilde{Z} = R + i\omega L + \frac{1}{i\omega C}.$$

Because our concern is the phase difference between current and voltage, we choose the phase angle for $\tilde{V}$ to be zero so that $\tilde{V} = V$, which is real. The complex current is

$$\tilde{I} = \frac{V}{\tilde{Z}};$$

we find the magnitude of the current to be

$$I = |\tilde{I}| = \frac{V}{\sqrt{R^2 + \left[(\omega L) - \left(\frac{1}{\omega C}\right)\right]^2}}, \tag{9.27}$$

with its phase angle relative to V,

$$\alpha_I = \arctan \frac{\frac{1}{\omega C} - \omega L}{R}. \tag{9.28}$$

The charge in the capacitor is

$$\tilde{q} = C\tilde{V}_C = C\tilde{I}\frac{1}{i\omega C};$$

therefore

$$q = |\tilde{q}| = \frac{V}{\sqrt{R^2\omega^2 + L^2(\omega^2 - \frac{1}{LC})^2}}. \tag{9.29}$$

Comparison of this result with oscillatory motion in a mechanical system indicates that charge corresponds to position; this expression is identical to equation (2.17) obtained from solving the differential equation:

$$x_{\max} = \frac{F_0}{\sqrt{b^2\omega^2 + m^2(\omega^2 - \frac{k}{m})^2}}.$$

The natural frequency for the system of spring and block is $\sqrt{k/m}$; when the driving frequency ω is set at the natural frequency the amplitude is extremely large. Analogously, for an RLC circuit driven by an alternating supply of power, its charge or current has a response curve identical to that of frequency; resonance occurs when the driving frequency is set equal to the natural frequency,

$$\omega = \omega_0 = \sqrt{\frac{1}{LC}}. \tag{9.30}$$

Worksheet 9.8 Maple provides the `abs` command to find the magnitude of a complex number, and the `argument` command to find the phase angle; these two commands are most useful for analysis of impedance circuits. We have already encountered the `evalc` command, which serves to simplify an expression containing complex numbers.

```
> assume(R>0, L>0, C>0, V0>0, omega>0):
> Z := R + I*omega*L + 1/(I*omega*C);
```

$$Z := R + \omega\, L\, I - \frac{I}{\omega\, C}$$

```
> current := V0/Z:
> current := evalc(current);
```

$$current := \frac{V0\ R}{R^2 + \left(\omega\, L - \frac{1}{\omega\, C}\right)^2} - \frac{V0\ \left(\omega\, L - \frac{1}{\omega\, C}\right)\ I}{R^2 + \left(\omega\, L - \frac{1}{\omega\, C}\right)^2}$$

```
> CurMag := abs(current):
> CurMag := simplify(CurMag);
```

$$CurMag := V0\,\omega\,C\sqrt{\frac{1}{R^2\,\omega^2\,C^2+\omega^4\,L^2\,C^2-2\,\omega^2\,L\,C+1}}$$

```
> CurPhase := argument(current);
```

$$CurPhase := \arctan\left(\frac{-\omega\,L+\frac{1}{\omega\,C}}{R}\right)$$

```
> charge := C*current*1/(I*omega*C);
```

$$charge := \frac{-I\left(\dfrac{V0\,R}{R^2+\left(\omega\,L-\dfrac{1}{\omega\,C}\right)^2}-\dfrac{V0\,\left(\omega\,L-\dfrac{1}{\omega\,C}\right)\,I}{R^2+\left(\omega\,L-\dfrac{1}{\omega\,C}\right)^2}\right)}{\omega}$$

```
> ChrMag := abs(charge):
> ChrMag := simplify(ChrMag);
```

$$ChrMag := V0\,C\sqrt{\frac{1}{R^2\,\omega^2\,C^2+\omega^4\,L^2\,C^2-2\,\omega^2\,L\,C+1}}$$

Example 9.6 A circuit shown in Figure 9.8, for which $R = 10$ kΩ, $C_1 = 0.5$ μF, $C_2 = 0.2$ μF, is driven by an alternating power supply for which $V = 120$ V and $f = 60$ Hz.[2] Find (a) the root-mean-square current and its phase of i_1, (b) the average power dissipated in the entire system, and (c) the root-mean-square voltage across the resistor.

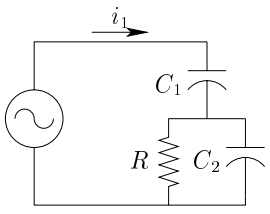


Figure 9.8: A network circuit.

Solution The angular frequency is

$$\omega = 2\pi f = 377\ (\mathrm{s}^{-1}).$$

[2]E. M. Purcell, *Electricity and Magnetism*, 2nd ed., New York: McGraw-Hill, 1985, p. 317.

The equivalent impedance for three elements combined is

$$\tilde{Z} = \frac{1}{i\omega C_1} + \frac{1}{\frac{1}{R} + i\omega C_2} = 6375.6 - 10112.2\,i.$$

We set $\tilde{V}$ to be real, so that

$$\tilde{I} = \frac{V}{\tilde{Z}}.$$

We use the root-mean-square value for V; the magnitude of $\tilde{I}$ automatically becomes a root-mean-square value. We have

$$\tilde{I} = \frac{120}{6375.6 - 10112.2i} = 0.0054 + 0.0085\,i.$$

We find the magnitude of current from

$$I_{\text{rms}} = |\tilde{I}| = 0.01\ (\text{A}),$$

which is i_1. The average power dissipated in the system is

$$\overline{P} = I_{\text{rms}}^2 \Re\{\tilde{Z}\} = (0.01)^2(6375.6) = 0.64\ (\text{W}).$$

The voltage across C_1 is

$$\tilde{I}\frac{1}{i\omega C_1} = 45.0 - 28.4\,i,$$

so the voltage across R (and C_2) is

$$120 - (45.0 - 28.4) = 74.9 + 28.4\,i,$$

of magnitude

$$|74.9 + 28.4\,i| = 80.2\ (\text{V}).$$

Worksheet 9.9 We apply the `abs` and `argument` commands to find the magnitude and phase angle of a complex number, respectively, and the `Re` command to extract the real part of a complex number.

```
> R := 10000; C1 := 0.5e-6; C2 := 0.2e-6; V0 := 120; omega :=
> 2*Pi*60;
```

$$R := 10000$$
$$C1 := 0.5\,10^{-6}$$
$$C2 := 0.2\,10^{-6}$$

$$V0 := 120$$

$$\omega := 120\,\pi$$

```
> Z := 1/(I*omega*C1) + 1/(1/R + I*omega*C2);
```

$$Z := -\frac{16666.66667\,I}{\pi} + \frac{1}{\frac{1}{10000} + 0.0000240\,I\,\pi}$$

```
> Z := simplify(evalc(Z));
```

$$Z := 6375.561852 - 10112.22516\,I$$

```
> current := V0/Z;
```

$$current := 0.005353682721 + 0.008491431245\,I$$

```
> crms := abs(current);
```

$$crms := 0.01003824304$$

```
> phaseangle := argument(current);
```

$$phaseangle := 1.008265605$$

```
> pow := crms^2*Re(Z);
```

$$pow := 0.6424419268$$

```
> VC1 := simplify(evalc(current*1/(I*omega*C1)));
```

$$VC1 := 45.04844188 - 28.40216896\,I$$

```
> VR := V0 - VC1;
```

$$VR := 74.95155812 + 28.40216896\,I$$

```
> VRmax := abs(VR);
```

$$VRmax := 80.15247511$$

9.4.2 Bridges

The Wheatstone bridge is applicable to an impedance circuit; the balance condition occurs on simply replacing the resistance R with the impedance $\tilde{Z}$,

$$\tilde{Z}_x = \frac{\tilde{Z}_2 \tilde{Z}_3}{\tilde{Z}_1}. \tag{9.31}$$

An impedance bridge is useful for measuring an unknown impedance. For instance, if one seeks to measure an unknown capacitance, to be designated C_x, one can use the bridge shown in Figure 9.9.

The impedances are

$$\tilde{Z}_1 = R_1, \quad \tilde{Z}_2 = R_2, \quad \tilde{Z}_3 = R_3 + \frac{1}{i\omega C_s}, \quad \tilde{Z}_x = R_x + \frac{1}{i\omega C_x}.$$

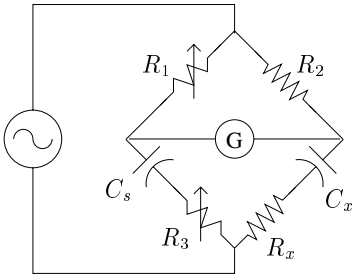


Figure 9.9: Bridge to compare capacitance.

Substituting these into the balance condition, we obtain

$$R_x + \frac{1}{i\omega C_x} = \frac{R_2\left(R_3 + \frac{1}{i\omega C_s}\right)}{R_1}.$$

Comparing real and imaginary parts, we find

$$R_x = \frac{R_2 R_3}{R_1}, \quad C_x = \frac{R_1 C_s}{R_2}. \tag{9.32}$$

Worksheet 9.10 The `Re` and `Im` commands serve to extract the real and imaginary parts of a complex number. For two complex numbers to be equal, both their real and imaginary parts must separately be equal.

```
> assume(R1, real, R2, real, R3, real, Rx, real, Cs, real, Cx,
real,
> omega, real):
> Z1 := R1;
```

$$Z1 := R1$$

```
> Z2 := R2;
```

$$Z2 := R2$$

```
> Z3 := R3 + 1/(I*omega*Cs);
```

$$Z3 := R3 - \frac{I}{\omega\, Cs}$$

```
> Z4 := Rx + 1/(I*omega*Cx);
```

$$Z4 := Rx - \frac{I}{\omega\, Cx}$$

```
> Eq1 := Z4 = Z2*Z3/Z1;
```

$$Eq1 := Rx - \frac{I}{\omega\, Cx} = \frac{R2\left(R3 - \frac{I}{\omega\, Cs}\right)}{R1}$$

```
> Eq2 := evalc(Eq1);
```

$$Eq2 := Rx - \frac{I}{\omega\, Cx} = \frac{R2\, R3}{R1} - \frac{R2\, I}{R1\, \omega\, Cs}$$

```
> Eq3 := Re(lhs(Eq2)) = Re(rhs(Eq2));
```

$$Eq3 := Rx = \frac{R2\, R3}{R1}$$

```
> Eq4 := Im(lhs(Eq2)) = Im(rhs(Eq2));
```

$$Eq4 := -\frac{1}{\omega\, Cx} = -\frac{R2}{R1\, \omega\, Cs}$$

```
> Eq5 := isolate(Eq4, Cx);
```

$$Eq5 := Cx = \frac{R1\, Cs}{R2}$$

See an exercise at the end of the chapter for another kind of impedance bridge, the Maxwell bridge, in which the standard capacitor is in parallel with a variable resistor. One can similarly obtain the values of R_x and L_x from the balance condition.

Exercises

1. In Section 9.1, we derive a formula for the delta-star transformation, which expresses R_a, R_b and R_c in terms of R_1, R_2 and R_3; see Figure 9.1. Conversely, we can derive the star-delta transformation: that is to find R_1, R_2 and R_3 in terms of R_a, R_b and R_c by solving the three equations of (9.4).

2. Referring to the Wheatstone bridge in Figure 9.2, let $R_3 = \alpha R_1$, $R_2 = \beta R_1$, then the balance condition gives $R_x = \alpha\beta R_1$. We want to determine the potential difference between a and b when R_1 is slightly changed, and also the value of α that results in the greatest potential difference.

   (a) If R_1 is changed to $R_1' = (1 + x)R_1$, provided x is small, then

   $$V_a - V_b = i_1 R_1' - i_2 R_2,$$

   where

   $$i_1 = \frac{V_s}{R_1' + R_3}, \quad i_2 = \frac{V_2}{R_2 + R_x}.$$

   Show that

   $$V \equiv \frac{V_a - V_b}{V_s} = \frac{\alpha x}{(1 + \alpha)(1 + \alpha + x)},$$

   which is independent of β. Make a plot of V as a function of x and α, which should resemble Figure 9.10.

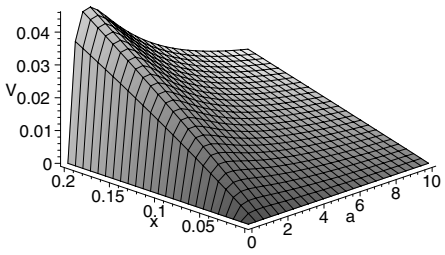


Figure 9.10: Potential difference as a function of α and x.

(b) With x fixed, at what value of α does V resume a maximum? This is the condition for maximum sensitivity.
Answer: $\alpha = \sqrt{1+x}$ ($\simeq 1$ for small x).

3. In Figure 9.4 (b), suppose that a capacitor is initially charged with q_0, and S_2 is closed at $t = 0$. Find charge q in the capacitor as a function of time, and plot this function.

4. Considering the RL circuit in Figure 9.5, suppose that switch S_1 has been closed for long enough so that the stable current is V_0/R. At one instant $t = 0$, S_2 is closed and S_1 is open. Find current as a function of time, and plot this function.

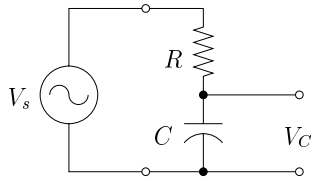


Figure 9.11: RC circuit.

5. For the circuit with $R = 1000\ \Omega$ and $C = 0.1$ μF shown in Figure 9.11, one sets the power supply to output a sine wave at 2000 Hz and 10 V. The voltage across the capacitor V_C is measured by an oscilloscope.

(a) On application of Kirchhoff's rule, the differential equation governing this system is

$$10\ \sin(2\pi f t) - \frac{dq(t)}{dt}R - \frac{q(t)}{C} = 0,$$

where $f = 2000$, $R = 1000$, and $C = 0.1 \times 10^{-6}$. Solve this equation for $q(t)$; the voltage across the capacitor is $q(t)/C$.

(b) Make a plot of both voltage of the source V_s and voltage across the capacitor V_C as functions of time, which resembles a display on an oscilloscope in the x–t mode;

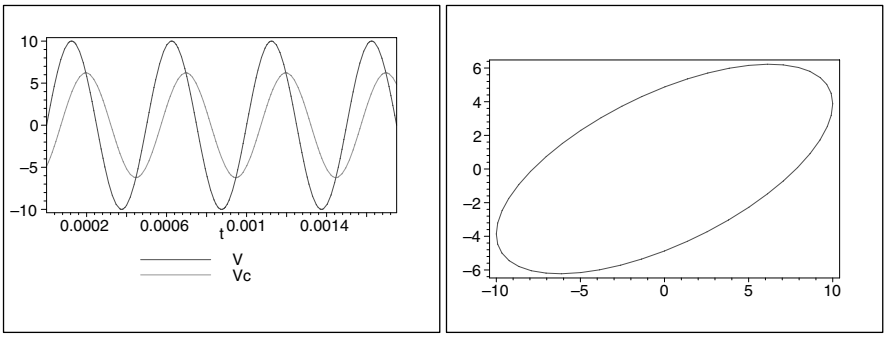


Figure 9.12: Display on an oscilloscope in x–t mode and x–y mode.

a phase difference should be noticed. Make another plot in parametric form of V_s and V_C, which resembles a display on an oscilloscope in the x–y mode, which is a Lissajous figure. Both results are displayed in Figure 9.12.

6. For a parallel RLC circuit in Figure 9.13 driven by an alternating power supply with root-mean-square voltage V_{rms} and angular frequency ω, find the root-mean-square current delivered by the source and its phase angle relative to the voltage.

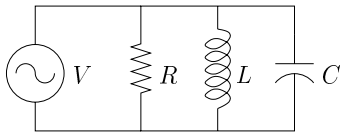


Figure 9.13: RLC circuit in parallel.

7. Figure 9.14 shows the Maxwell bridge; from the balance condition, find R_x and L_x in terms of known components R_1, R_2, R_3 and C_s.

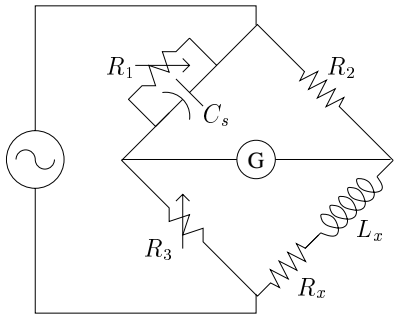


Figure 9.14: Maxwell bridge.

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10 Waves

In this chapter we introduce wave phenomena. This topic gives us the opportunity to integrate mathematical skills acquired in solving partial differential equations and expanding functions in Fourier series and integrals, introduced mainly in Chapters 5 and 7. Knowledge of waves is important in our treatment of quantum mechanics in subsequent chapters. We also discuss the generation of electromagnetic waves through electric-dipole radiation, which is an example of solving the time-dependent Maxwell equations. Electromagnetic waves are the foundation of our treatment of physical optics in the next chapter. A wave is described by a function of space and time, in which Maple can produce animations so that we can visualize the motion.

10.1 Wave Equation

Mathematically, a wave is a function of space and time that satisfies this equation,

$$\nabla^2\psi = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2}, \tag{10.1}$$

which is a partial differential equation of second order in space and second order in time; v denotes the wave velocity. Many physical phenomena related to oscillation can be described by waves. For example, a wave equation can describe the surface of a water wave, or sound, which is the oscillation of air density.

In one dimension, the wave equation is

$$\frac{\partial^2\psi(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2\psi(x,t)}{\partial t^2}. \tag{10.2}$$

We use Maple to solve this one-dimensional wave equation.

Worksheet 10.1 A partial differential equation is generally difficult to solve; Maple has a command `pdsolve` for this purpose.

```
> Eq1 := diff(psi(x,t), x$2) = 1/v^2*diff(psi(x,t), t$2);
```

$$Eq1 := \frac{\partial^2}{\partial x^2}\psi(x,\,t) = \frac{\frac{\partial^2}{\partial t^2}\psi(x,\,t)}{v^2}$$

Physics with Maple™: The Computer Algebra Resource for Mathematical Methods in Physics. Frank Y. Wang
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ISBN: 3-527-40640-9

```
> Soln1 := pdsolve(Eq1, psi(x,t));
```

$$Soln1 := \psi(x,\, t) = _\mathrm{F1}(v\,t + x) + _\mathrm{F2}(v\,t - x)$$

According to Maple output with slight modification, the solution of the one-dimensional wave equation is expressed in the general form,

$$\psi(x,t) = F(x - vt) + G(x + vt), \tag{10.3}$$

which is d'Alembert's solution.

In equation (10.3), F represents a wave propagating in the positive x direction with speed v, whereas G is a wave propagating in the negative x direction. We invoke Maple's `animate` command to illustrate wave motion. An animation consists of plot frames displayed one after another, sequentially. Displaying animation in a book is difficult because a still picture fails to convey the dynamic behavior. The reader should enter these commands into a Maple session to enhance their understanding.

Example 10.1 Observe the motion of the wave functions

$$\psi(x,t) = 5.0\, e^{-(x-3.0t)^2}$$

and

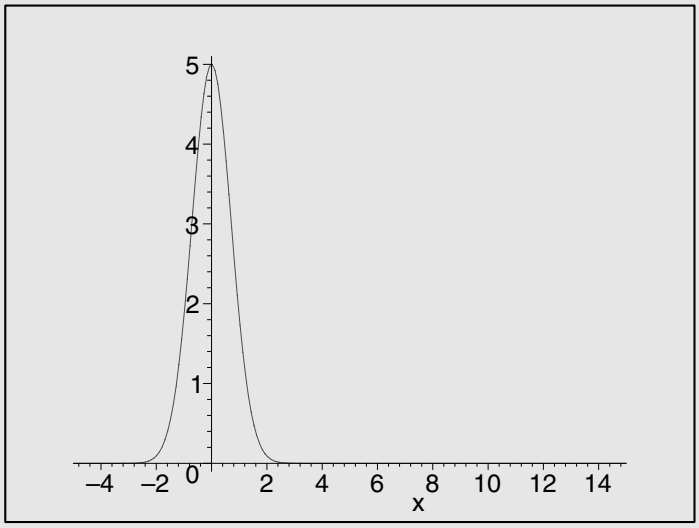
$$\psi(x,t) = 5.0\, e^{-(x+3.0t)^2}.$$

Solution We can produce an animation by directly entering the wave function under the `animate` command.

Worksheet 10.2 The `animate` command is straightforward. If we alter the sign of v in the worksheet to $+3.0$, we can generate the other type of solution of the wave equation, which propagates in the negative x direction.

```
> with(plots):

Warning, the name changecoords has been redefined
> animate(plot, [5.0*exp(-(x-3.0*t)^2), x=-5..15], t=0..3,
numpoints=200);
```



In this worksheet we display a still picture at one instant. We call this function of space $\psi(x, t_0)$ the wave profile.

The most familiar wave has a sinusoidal profile, which is a plane wave. Such a wave is characterized by wavelength λ and period T, and is described mathematically as

$$\psi(x,t) = A\sin(kx - \omega t + \delta), \tag{10.4}$$

where δ is the phase angle. The cosine serves equally well for this purpose. In this equation, k is the wave number that is related to the wavelength λ as

$$k = \frac{2\pi}{\lambda}, \tag{10.5}$$

and the angular frequency ω is related to the period T as

$$\omega = \frac{2\pi}{T}. \tag{10.6}$$

Because this function must satisfy a general solution for the wave, ω and k are related by

$$\omega = kv, \tag{10.7}$$

where v is the phase velocity of the wave.

Example 10.2 Observe the motion of these three functions:

$$f_1 = \sin(x - t),$$
$$f_2 = \sin(x + t),$$
$$f_3 = f_1 + f_2.$$

Solution An animation is readily produced on entering these functions directly; we omit the output plots.

Worksheet 10.3

```
> with(plots):
> f1 := sin(x-t);
> f2 := sin(x+t);
> animate(plot, [f1, x=-4*Pi..4*Pi], t=0..4*Pi);
> animate(plot, [f2, x=-4*Pi..4*Pi], t=0..4*Pi);
> p1 := animate(plot, [f1, x=-4*Pi..4*Pi, color=blue], t=0..2*Pi,
numpoints=200, thickness=1):
> p2 := animate(plot, [f2, x=-4*Pi..4*Pi, color=yellow], t=0..2*Pi,
numpoints=200, thickness=1):
> p3 := animate(plot, [f1+f2, x=-4*Pi..4*Pi, color=green],
t=0..2*Pi, numpoints=200, thickness=2):
> display([p1, p2, p3]);
```

Running this animation, one can observe the behavior of wave f_3, which is formed on adding f_1, a wave traveling to the right, and f_2, a wave traveling to the left. It appears that f_3 does not propagate; it simply oscillates up and down in a fixed pattern. The mathematical formula for the composite wave f_3 is

$$\sin[k(x - vt)] + \sin[k(x + vt)] = 2\sin(kx)\cos(kvt). \tag{10.8}$$

Worksheet 10.4

```
> f1:=sin(k*(x-v*t)); f2:=sin(k*(x+v*t));
```

$$f1 := \sin(k\,(x - v\,t))$$

$$f2 := \sin(k\,(x + v\,t))$$

```
> f3 := f1 + f2:
> expand(f3);
```

$$2\sin(k\,x)\cos(k\,v\,t)$$

According to this formula, at any fixed x, the wave oscillates with frequency $\omega = kv$ and amplitude $2\sin(kx)$. We refer to this characteristic as a mode, which is a pattern of motion that at any point moves sinusoidally, and for which all points move at the same frequency. The amplitude of a mode vanishes at points for which $\sin(kx) = 0$, that is,

$$x = 0, \frac{\pi}{k}, \frac{2\pi}{k}, \frac{3\pi}{k}, \ldots;$$

these points are nodes. The distance between successive nodes is π/k, which is half a wavelength for the corresponding mode. Complicated motion can be analyzed by combining various modes, which we will discuss in the next section.

10.2 Vibrating String

We consider the physics of a vibrating string, that is, a wave on a string of length l, fastened at both ends $x = 0$ and $x = l$. Such a situation is commonly observable for some musical instruments, for instance, a violin string. To describe motion of a wave under these conditions, we seek to find the solution of the wave equation,

$$\frac{\partial^2 \psi(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 \psi(x,t)}{\partial t^2}, \tag{10.9}$$

which is subject to the boundary conditions,

$$\psi(0,t) = 0, \quad \psi(l,t) = 0, \quad t \geq 0. \tag{10.10}$$

Moreover, suppose that the string is plucked from its null position $f(x)$ and released with a velocity $g(x)$ at time $t = 0$, so that this string begins to vibrate. We impose the corresponding initial conditions,

$$\psi(x,0) = f(x), \tag{10.11}$$

and

$$\left.\frac{\partial \psi}{\partial t}\right|_{t=0} = g(x). \tag{10.12}$$

Separation of variables, discussed in Chapter 7, is the method that we apply to solve this problem. Let $\psi(x,t) = X(x)T(t)$, and assign a constant $-n^2k^2$ after separation of variables; the solution for the spatial equation is

$$X(x) = \sin(nkx),$$

and for the temporal equation,

$$T(t) = a\cos(nkvt) + b\sin(nkvt).$$

Because the spatial solution is subject to boundary conditions, of which one is $X(l) = 0$, we must have

$$nkl = n\pi, \quad k = \frac{\pi}{l}. \tag{10.13}$$

The general solution is a linear combination of terms with various n,

$$\psi(x,t) = \sum_{n=1}^{\infty} \sin(nkx)[a_n \cos(nkvt) + b_n \sin(nkvt)]. \tag{10.14}$$

This solution is a combination of modes, each characterized by an integer n. This solution reflects an important principle of a linear system: any motion can be expressed as an expansion in distinct modes. The frequency corresponding to a mode is $n\omega = nkv$, which can only occur at certain discrete values. The condition $n = 1$ denotes the fundamental frequency; $n > 1$ denotes a harmonic, which can only be an integer multiple of the fundamental frequency. For this general form, coefficients a_n and b_n are simply obtained as Fourier coefficients:

$$a_n = \frac{2}{l}\int_0^l f(x)\sin(nkx)\,dx, \tag{10.15a}$$

$$b_n = \frac{2}{nkvl}\int_0^l g(x)\sin(nkx)\,dx. \tag{10.15b}$$

Be aware of a subtle difference of the definition of k between these equations and the Fourier series in Section 5.1, because, for the fundamental mode, the distance between the nodes is l, which is half a wavelength. We can regard $f(x)$ and $g(x)$ as odd functions with period $\lambda = 2l$, such that $f(x + 2l) = f(x)$.

Example 10.3 A string of length $l = 3$ is disturbed at $t = 0$ with an initial displacement

$$f(x) = \begin{cases} x & 0 < x < 1, \\ \dfrac{3}{2} - \dfrac{x}{2} & 1 < x < 3; \end{cases} \tag{10.16}$$

there is no initial velocity. Find the wave function $\psi(x, t)$ for $t > 0$.

Solution We have evaluated the Fourier coefficients of a similar function in Section 5.1; in that problem the function is a full wave, so $L = 3$, but here it is a half wave, so $l = 3$ and $\lambda = 2l = 6$. Therefore k differs by a factor of 2:

$$a_n = \frac{2}{l}\int_0^l f(x)\sin(nkx)\,dx.$$

The integrals are readily evaluated with Maple, which yields the result

$$\psi(x,t) = \frac{9\sqrt{3}}{2\pi^2}\sin\frac{\pi x}{3}\cos\frac{\pi vt}{3} + \frac{9\sqrt{3}}{8\pi^2}\sin\frac{2\pi x}{3}\cos\frac{2\pi vt}{3} - \frac{9\sqrt{3}}{32\pi^2}\sin\frac{4\pi x}{3}\cos\frac{4\pi vt}{3} - \frac{9\sqrt{3}}{50\pi^2}\sin\frac{5\pi x}{3}\cos\frac{5\pi vt}{3} + \ldots.$$

Worksheet 10.5 We evaluate the coefficients, employing the exact method of Chapter 5. We animate the wave motion described by ψ, which is a function of x and t, using the `animate` command.

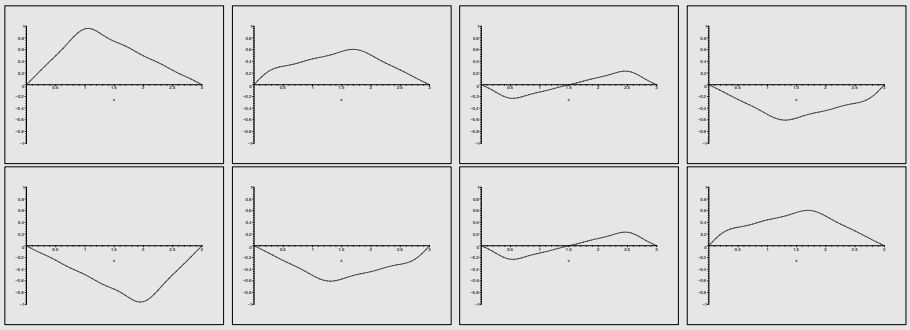
```
> L := 3:  v := 1:
> k := Pi/L;
```

$$k := \frac{\pi}{3}$$

```
> N := 10:
> for n from 1 to N do
> L := 3:  v := 1:
> k := Pi/L;
```

$$k := \frac{\pi}{3}$$

```
> N := 10:
> for n from 1 to N do
> a[n] := 2/L*(int(x*sin(n*k*x), x=0..1)
> + int((3/2 - x/2)*sin(n*k*x), x=1..3)):
> end do:
> n := 'n':
> Epr2 := add(a[n]*sin(n*k*x)*cos(n*k*v*t), n=1..N):
> with(plots):
Warning, the name changecoords has been redefined
> animate(plot, [Epr2, x=0..L], t=0..6, scaling=constrained);
```



Most partial differential equations admit no analytic solution; thus we must resort to numerical methods. Numerical solution of a partial differential equation involves more complicated techniques; a widely used one is the finite-difference method. Commercial programs are available to solve partial differential equations numerically, and Maple implements some algorithms. The reader might obtain information from help under `pdsolve[numeric]`; this command accepts only certain types of boundary-value problems and is subject to improvement. A vibrating string is one type of problem suitable for `pdsolve` with option `numeric`; we present the worksheet below. Because application of this command is limited at this stage, we do not explore this topic any further.

Worksheet 10.6

```
> Eq1 := diff(psi(x,t), x$2) = diff(psi(x,t), t$2);
> Eq2 := {psi(0, t)=0, psi(3, t)=0};
> Eq3 := {psi(x, 0)= piecewise( x >= 0 and x <= 1, x, x > 1 and x
<= 3, 3/2-x/2), D[2](psi)(x,0)=0};
> Soln1 := pdsolve(Eq1, Eq2 union Eq3, numeric);
> Soln1:-animate( psi(x,t) ,t=0..2*Pi, scaling=constrained);
```

10.3 Sinusoidal Waves in Linear Combinations

The result of the preceding section indicates that a wave confined to $0 < x < l$, or a periodic wave $\psi(x + l, t) = \psi(x, t)$, can be expressed as sinusoidal waves in linear combination, which is the Fourier series listed in equation (10.14). For given initial position and velocity, the Fourier coefficients are evaluated according to equation (10.15).

We extend this concept to any wave that satisfies the wave equation in a domain $-\infty < x < \infty$; such an extension is naturally a Fourier integral. Before discussing this topic, we define our prospective notation; we then introduce an important theorem: the uncertainty principle related to the Fourier integral.

10.3.1 Complex Notation

Exponentials are generally easier to manipulate than sines and cosines. Euler's formula

$$e^{i\theta} = \cos\theta + i\sin\theta \tag{10.17}$$

relates these functions so that we can express a sinusoidal wave in complex notation. We have shown how to use complex numbers for an electric circuit, and the advantage of using complex numbers becomes further evident in Section 11.2; we devote this section to notation because it is sometimes a source of confusion.

A sinusoidal wave has the general form

$$\psi(x, t) = A\cos(kx - \omega t + \delta), \tag{10.18}$$

where δ is the phase angle. According to Euler's formula, this can be written as

$$\psi(x, t) = \Re\left\{Ae^{i(kx-\omega t+\delta)}\right\}. \tag{10.19}$$

We introduce a notation for a complex wave function, indicated by tilde,

$$\tilde{\psi}(x,t) = \tilde{A}e^{i(kx-\omega t)}, \tag{10.20}$$

and

$$\tilde{A} = Ae^{i\delta}. \tag{10.21}$$

The complex amplitude $\tilde{A}$ absorbs the phase angle; hence it contains information of both amplitude A and phase angle δ, both real numbers. We can find the magnitude of the amplitude as a complex scalar product of $\tilde{A}$ with itself,

$$A^2 = \tilde{A}\tilde{A}^*, \quad A = \sqrt{A^2}. \tag{10.22}$$

Because measurement of a physical quantity yields a real number, our interest typically lies in the real part of a complex wave function,

$$\psi(x,t) = \Re\{\tilde{\psi}(x,t)\}. \tag{10.23}$$

In some literature, a wave function in complex notation is written without a tilde; such an omission might result in confusion between A and $\tilde{A}$. In this and the next chapter we make an effort to distinguish a complex number from its magnitude, which is a real number, by deploying a tilde to denote the former. One should be aware that, for a sinusoidal wave expressed in complex notation, the amplitude should always be regarded as a complex number. In the case when the tilde is lacking, the complex amplitude A can be expressed in the polar form,

$$A = |A|e^{i\delta}.$$

Some authors intend this expression for equation (10.21): one should exercise due care with notation.

10.3.2 Fourier Integrals

A wave $\psi(x,t)$ in a domain $-\infty < x < \infty$ can be represented as a Fourier integral,

$$\psi(x,t) = \frac{1}{(2\pi)^{1/2}}\Re\left\{\int_{-\infty}^{\infty}\tilde{\alpha}(k)e^{ikx-\omega t}dk\right\}, \tag{10.24}$$

where $\tilde{\alpha}(k)$ is the Fourier transform; we here employ the complex notation.

Similar to a problem in Fourier series, if we are supplied initial conditions, such as initial position and velocity at $t = 0$,

$$\psi(x,0) = f(x), \tag{10.25}$$

and

$$\left.\frac{\partial\psi}{\partial t}\right|_{t=0} = g(x), \tag{10.26}$$

we can calculate the Fourier transform,

$$\tilde{\alpha}(k) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \left[f(x) + \frac{i}{\omega} g(x) \right] e^{-ikx}\, dx. \tag{10.27}$$

One should find the analogy between this equation and equation (10.15), for which we omit the derivation.

We mention above in relation to equation (10.7) that, for a sinusoidal wave, the wave velocity is

$$v = \frac{\omega}{k}.$$

This velocity v is called the phase velocity. In a dispersive medium the phase velocity varies for each frequency component of the wave; ω and k are thus not independent variables. We write the angular frequency ω as a function of the wave number k,

$$\omega = \omega(k). \tag{10.28}$$

Because ω depends on k, it must remain inside the integral in equation (10.24).

10.3.3 Uncertainty Principle

Although the uncertainty principle is often regarded to be of a quantum nature, it is actually a property of any wave, related to the Fourier integral.

An infinitely long periodic wave with a constant amplitude, such as $A\sin(k_0 x)$, is a featureless carrier that cannot transmit information. To transmit information, we must truncate the wave to form a finite wave train of length Δx. The speed with which this wave train propagates is called the group velocity. In a dispersive medium, we define the group velocity as

$$v_{\mathrm{g}} = \frac{d\omega(k)}{dk}. \tag{10.29}$$

This quantity typically differs from the phase velocity, which is ω/k.

Like any other wave, a wave train can be represented as a linear combination of many sinusoidal waves of wave number k; the amplitude of each sinusoidal wave is just the Fourier transform $\tilde{\alpha}(k)$. We make an observation of two functions and their Fourier transforms. To simplify our discussion, in this section the initial velocity $g(x)$ is of no concern.

Example 10.4 We have a wave $\cos(k_0 x)$ enveloped through these two functions:

$$f_1(x) = \begin{cases} 1, & -\dfrac{1}{2} < x < \dfrac{1}{2}, \\ 0, & x < -\dfrac{1}{2}, \quad \dfrac{1}{2} < x, \end{cases}$$

and

$$f_2(x) = \begin{cases} 2, & -\dfrac{1}{4} < x < \dfrac{1}{4}, \\ 0, & x < -\dfrac{1}{4}, \quad \dfrac{1}{4} < x. \end{cases}$$

Find their Fourier transforms.

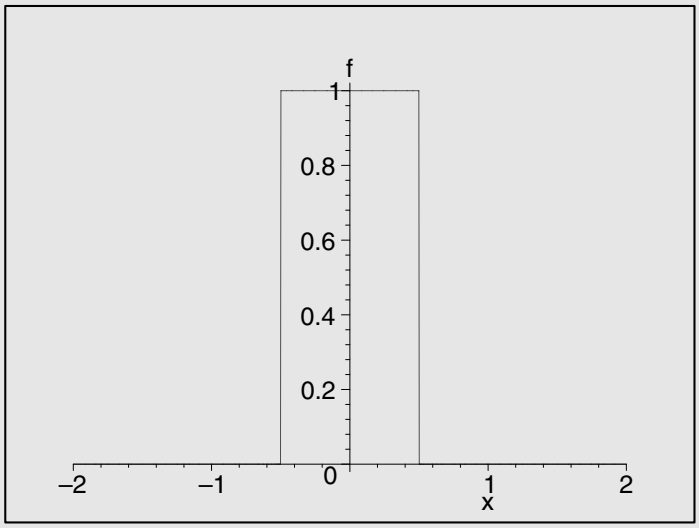
Solution Without loss of generality, the wave number k_0 can be set to an arbitrary value; for convenience we set it to zero. We have performed Fourier transformation of this type in Section 5.2:

$$\tilde{\alpha}(k) = \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} e^{-kx}\, dx = \sqrt{\frac{2}{\pi}} \frac{\sin ka}{k}. \tag{10.30}$$

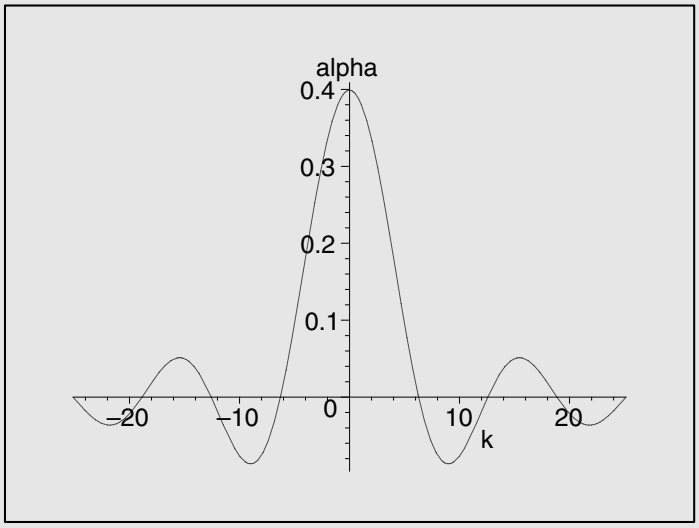
We display the graphical output.

Worksheet 10.7 The Fourier transform and its plot can be conveniently produced by Maple with the `int` and `plot` commands.

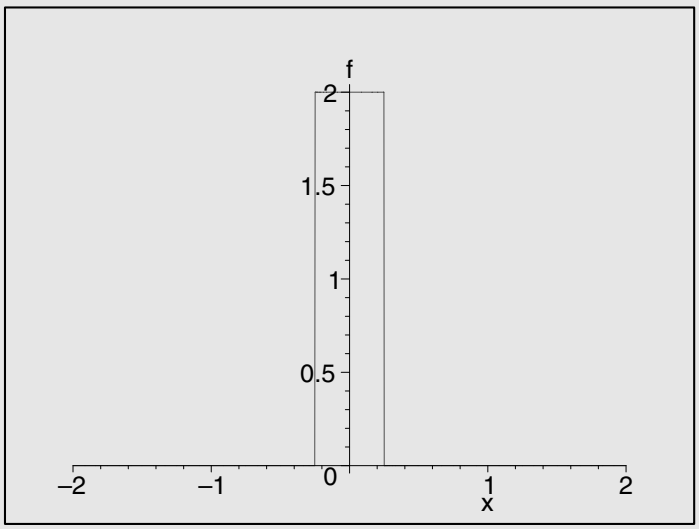
```
> f1 := piecewise(-1/2<x and x<1/2, 1, x<-1/2, 0, 1/2<x, 0):
> plot(f1,x=-2..2);
```



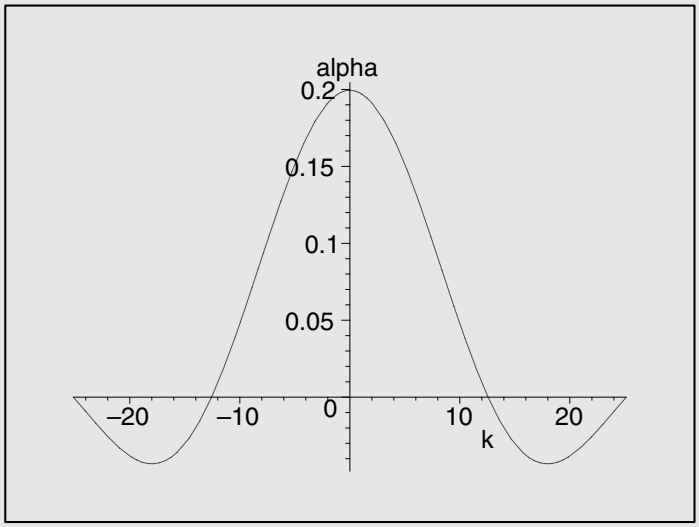
```
> g1 := 1/sqrt(2*Pi)*int(1*exp(-I*k*x), x=-1/2..1/2):
> g1 := simplify(g1):
> plot(g1,k=-8*Pi..8*Pi);
```




```
> f2 := piecewise(-1/4<x and x<1/4, 2, x<-1/4, 0, 1/4<x, 0):
> plot(f2,x=-2..2);
```




```
> g2 := 1/sqrt(2*Pi)*int(1*exp(-I*k*x), x=-1/4..1/4):
> g2 := simplify(g2):
> plot(g2,k=-8*Pi..8*Pi);
```



From the plots in the worksheet, we see that Fourier transform $\tilde{\alpha}(k)$ is a function with a maximum at k_0 (which we set to zero) and breadth of order Δk. The sharper the function, the broader its Fourier transform. Before we define Δx and Δk exactly, we estimate their orders of magnitude from the graph. For the first function, $\Delta x \sim 1/2$ and $\Delta k \sim 2\pi$ (the symbol $\sim$ denotes an estimate of order of magnitude), and for the second function, $\Delta x \sim 1/4$ and $\Delta k \sim 4\pi$. We see a trend that

$$\Delta x \Delta k \sim \pi.$$

To state this result quantitatively, we define the root-mean-square deviations of the position and the wave number as

$$\overline{x} = \frac{\int_{-\infty}^{\infty}(f^* x f)\,dx}{\int_{-\infty}^{\infty}(f^* f)\,dx}, \quad \overline{x^2} = \frac{\int(f^* x^2 f)\,dx}{\int(f^* f)\,dx}, \quad \Delta x = \left(\overline{x^2} - \overline{x}^2\right)^{1/2}, \tag{10.31a}$$

$$\overline{k} = \frac{\int_{-\infty}^{\infty}(\tilde{\alpha}^* k \tilde{\alpha})\,dk}{\int_{-\infty}^{\infty}(\tilde{\alpha}^* \tilde{\alpha})\,dk}, \quad \overline{k^2} = \frac{\int(\tilde{\alpha}^* k^2 \tilde{\alpha})\,dk}{\int(\tilde{\alpha}^* \tilde{\alpha})\,dk}, \quad \Delta k = \left(\overline{k^2} - \overline{k}^2\right)^{1/2}, \tag{10.31b}$$

respectively, where f^* and $\tilde{\alpha}^*$ are complex conjugates of the position function and its Fourier transform.

For any wave function, there is an uncertainty relation,

$$\boxed{\Delta x\, \Delta k \geq \frac{1}{2}}. \tag{10.32}$$

Instead of a proof of this property, we offer an example. The equality sign applies to the Gaussian function; we perform a calculation for such a function.

Example 10.5 A Gaussian function is defined as

$$f(x) = \frac{1}{\sqrt{2\pi}a} e^{-\frac{x^2}{2a^2}}, \tag{10.33}$$

where a characterizes the width of the profile. Find the Fourier transform of a sinusoidal wave enveloped by this function, and verify the uncertainty relation.

Solution Again we set the wave number $k_0 = 0$. The Fourier transform of a Gaussian function is

$$\alpha(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f e^{-ikx}\, dx = \frac{1}{\sqrt{2\pi}} e^{-\frac{a^2k^2}{2}}. \tag{10.34}$$

This Fourier transform is also a Gaussian function, but a appears in the numerator, not the denominator. We use the definition in equation (10.31) to find the root-mean-square deviation. From symmetry, $\overline{x}$ and $\overline{k}$ are zero. We have

$$\overline{x^2} = \frac{\int_{-\infty}^{\infty} (f x^2 f) dx}{\int_{-\infty}^{\infty} (f^2) dx} = \frac{a^2}{2},$$

and

$$\overline{k^2} = \frac{\int_{-\infty}^{\infty} (\alpha k^2 \alpha) dk}{\int_{-\infty}^{\infty} (\alpha^2) dk} = \frac{1}{2a^2};$$

therefore,

$$\Delta x\, \Delta k = \frac{1}{2}.$$

Worksheet 10.8 Basic Gaussian integrals can be readily evaluated by Maple.

```
> assume(a>0);
> f := 1/(sqrt(2*Pi)*a)*exp(-x^2/(2*a^2));
```

$$f := \frac{1}{2} \frac{\sqrt{2}\, e^{(-\frac{x^2}{2\,a^2})}}{\sqrt{\pi}\, a}$$

```
> g := 1/sqrt(2*Pi)*int(f*exp(-I*k*x), x=-infinity..infinity);
```

$$g := \frac{1}{2} \frac{\sqrt{2}\, e^{(-\frac{a^2\,k^2}{2})}}{\sqrt{\pi}}$$

```
> xsq := int((f*x)^2, x=-infinity..infinity)/int(f^2,
x=-infinity..infinity);
```

$$xsq := \frac{a^2}{2}$$

```
> ksq := int((g*k)^2, k=-infinity..infinity)/int(g^2,
k=-infinity..infinity);
```

$$ksq := \frac{1}{2\,a^2}$$

```
> Epr1 := sqrt(xsq)*sqrt(ksq);
```

$$Epr1 := \frac{1}{2}$$

When we replace x with t, and k with ω, we obtain the uncertainty relation in the domain of time and frequency,

$$\Delta t\,\Delta\omega \geq \frac{1}{2}. \tag{10.35}$$

Suppose that we seek to approximate a pulse, which is a wave train of finite duration, by sinusoidal waves; the briefer the time interval, the broader the frequency required. This uncertainty relation plays a crucial role in communication. The limiting speed of data transmission is determined by the duration of each piece of the signal: the smaller Δt, the more information can be delivered in unit time. To abbreviate a pulse, one must increase the bandwidth $\Delta\omega$.

In quantum mechanics, the frequency is energy divided by the Planck constant h, and the wave number is the momentum divided by the Planck constant. Thus the uncertainty principle of Heisenberg is related to the wave property of matter; we will discuss this topic in Chapters 13 and 14.

10.4 Gaussian Wave Packet

A Gaussian wave packet is a sinusoidal wave at a particular wavelength modulated by a Gaussian function, defined in the preceding section; we write it as

$$f(x) = e^{-\frac{x^2}{2a^2}} \cos(k_0 x). \tag{10.36}$$

Using complex notation for convenience, we express $f(x)$ as

$$f(x) = \Re\left\{e^{-\frac{x^2}{2a^2}} e^{ik_0 x}\right\}. \tag{10.37}$$

To find the time evolution of a Gaussian wave packet, we express it in terms of a Fourier integral. The calculation of the Fourier transform is straightforward:

$$\tilde{\alpha}(k) = a e^{\frac{-a^2}{2}(k-k_0)^2}. \tag{10.38}$$

To express the wave as a Fourier integral, we must specify $\omega = \omega(k)$. According to a common model,[1] ω depends on k to the quadratic power:

$$\omega = \omega_0 \left(1 + \frac{b^2 k^2}{2}\right). \tag{10.39}$$

With this ω, we express the wave with its time evolution as a Fourier integral:

$$\psi(x,t) = \frac{a}{(2\pi)^{1/2}} \Re \left\{ \int_{-\infty}^{\infty} \left[e^{\frac{-a^2}{2}(k-k_0)^2} \right] e^{i[kx - \omega_0(1+b^2k^2/2)t]} dk \right\}. \tag{10.40}$$

Maple can evaluate this integral exactly (see worksheet); we omit listing the result because in quantum mechanics we will again consider a Gaussian wave packet. The result is still a wave modulated with a Gaussian function, moving at group velocity

$$v_{\mathrm{g}} = \left. \frac{d\omega(k)}{dk} \right|_{k=k_0} = \omega_0 b^2 k_0. \tag{10.41}$$

The width of the Gaussian function is

$$a(t) = a \left[1 + \left(\frac{b^2 \omega_0 t}{a^4} \right)^2 \right]^{1/2}, \tag{10.42}$$

which increases with time. From the animation, we can observe that the Gaussian wave packet "diffuses" when propagating in a dispersive medium.

Worksheet 10.9 We use Maple to evaluate Gaussian integrals; we plot the wave function $\psi(x,t)$ in a three-dimensional graph, and produce an animation.

```
> assume(a>0, b>0, omega0>0, t>0);
> f := exp(-x^2/(2*a^2))*exp(I*k0*x);
```

$$f := e^{(-\frac{x^2}{2\,a^2})}\, e^{(k0\,x\,I)}$$

```
> alpha := 1/sqrt(2*Pi)*int(f*exp(-I*k*x), x=-infinity..infinity);
```

$$\alpha := e^{(-\frac{a^2\,(-k0+k)^2}{2})}\, a$$

```
> omega := omega0*(1 + 1/2*b^2*k^2);
```

$$\omega := \omega 0 \left(1 + \frac{b^2\,k^2}{2}\right)$$

[1] The interested reader might consult Jackson 1999, Sections 7.8 and 7.9 for the spreading of a pulse as it propagates in a dispersive medium.

```
> psi := 1/sqrt(2*Pi)*int(alpha*exp(I*(k*x-omega*t)),
> k=-infinity..infinity);
```

$$\psi := \frac{\sqrt{2}\, e^{\left(\frac{-1/2\, I\, (a^2\, k0^2\, \omega 0\, t\, b^2 + 2\, \omega 0\, t\, a^2 + 2\, I\, \omega 0^2\, t^2\, b^2 - 2\, a^2\, k0\, x - x^2\, I)}{a^2 + \omega 0\, t\, b^2\, I}\right)} a}{\sqrt{2\, a^2 + 2\, I\, \omega 0\, t\, b^2}}$$

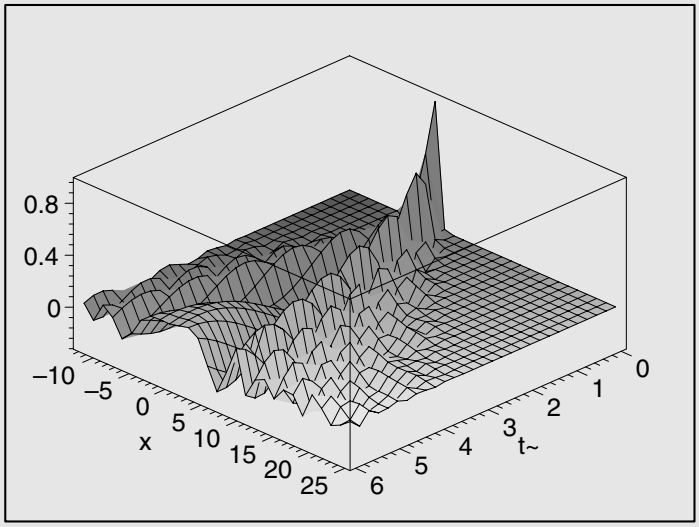
```
> psi1 := eval(Re(psi), {a=0.5, b=1, omega0=1, k0=1});
```

$$\psi 1 := 0.5\, \sqrt{2}\, \Re \left(\frac{e^{\left(\frac{-1/2\, I\, (0.75\, t + 2\, I\, t^2 - 0.50\, x - x^2\, I)}{0.25 + t\, I}\right)}}{\sqrt{0.50 + 2\, I\, t}} \right)$$

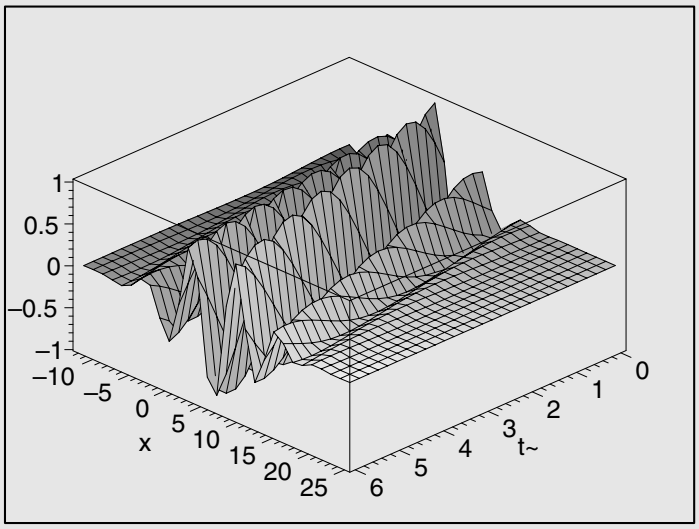
```
> psi2 := eval(Re(psi), {a=5, b=1, omega0=1, k0=1});
```

$$\psi 2 := 5\, \sqrt{2}\, \Re \left(\frac{e^{\left(\frac{-1/2\, I\, (75\, t + 2\, I\, t^2 - 50\, x - x^2\, I)}{25 + t\, I}\right)}}{\sqrt{50 + 2\, I\, t}} \right)$$

```
> plot3d(Re(psi1), t=0..6, x=-12..25, axes=boxed, numpoints=800);
```



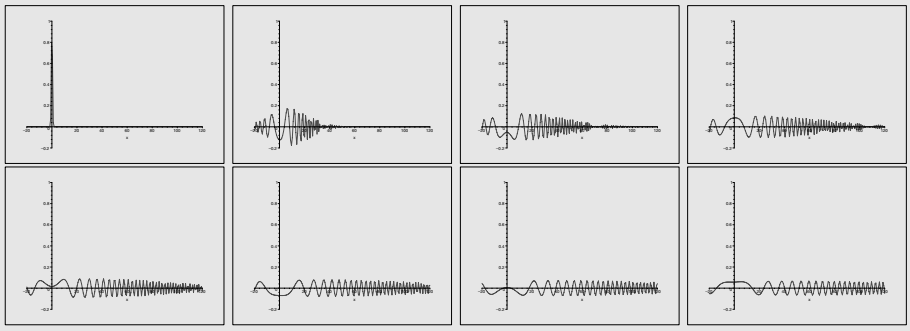

```
> plot3d(Re(psi2), t=0..6, x=-12..25, axes=boxed, numpoints=800);
```



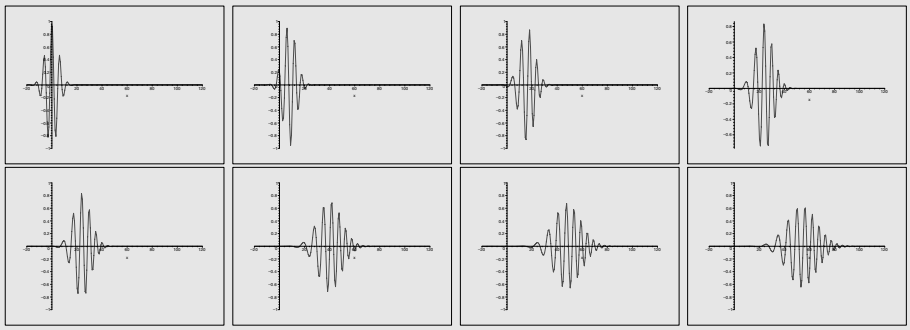

```
> with(plots):
```

```
Warning, the name changecoords has been redefined
```

```
> animate(plot, [Re(psi1), x=-20..120], t=0..60, numpoints=200);
```



```
> animate(plot, [Re(psi2), x=-20..120], t=0..60, numpoints=200);
```



According to these plots, the shape of the wave profile varies as it propagates. The broad packet ($k_0 a \gg 1$) distorts slowly, but the narrow packet ($k_0 a \lesssim 1$) broadens rapidly.

10.5 Two-dimensional Circular Membrane

The wave equation in three dimensions is

$$\nabla^2 \psi = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2}. \tag{10.43}$$

The Laplacian ∇^2 can be expressed in various coordinate systems, as we have examined in Chapter 7. Most techniques for solving a partial differential equation related to the Laplacian introduced in the theory of potential are applicable to wave equations.

In this section we consider a two-dimensional circular membrane, such as a drum. It is appropriate to use polar coordinates ρ and ϕ, which can be considered as cylindrical coordinates without the z component. Modifying the formulation in Section 7.6 in which we discuss the Laplace equation in cylindrical coordinates, we directly obtain a solution of the wave equation in polar coordinates. A differential equation to describe the oscillatory motion of the two-dimensional circular membrane is

$$\frac{\partial^2 \psi}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \psi}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \phi^2} = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2}, \tag{10.44}$$

where ψ is a function of ρ, ϕ and t,

$$\psi = \psi(\rho, \phi, t).$$

As the surface of the drum is fixed at $\rho = a$, the radius of the drum, the boundary condition is

$$\psi(a, \phi, t) = 0. \tag{10.45}$$

When the drum is excited by an initial displacement, the initial condition is

$$\psi(\rho, \phi, 0) = f(\rho, \phi). \tag{10.46}$$

We suppose that there is no initial velocity, although to include such a contribution is not difficult.

To solve this equation, we again apply the technique of separation of variables, letting $\psi = R(\rho)\Phi(\phi)T(t)$; we adopt results directly from the Laplace equation in cylindrical coordinates in Section 7.6. Comparing equation (10.44) with the boundary-value problem for the potential in cylindrical coordinates,

$$\frac{\partial^2 V}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial V}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 V}{\partial \phi^2} + \frac{\partial^2 V}{\partial z^2} = 0, \tag{10.47}$$

we find the only difference to be

$$\frac{\partial^2 V}{\partial z^2} \to -\frac{1}{v^2}\frac{\partial^2 \psi}{\partial t^2}.$$

We thus replace Z with T as

$$Z(z) = \sinh(kz) \to T(t) = \cos(kvt).$$

The angular and radial solutions are the same,

$$\Phi(\phi) = A\sin(m\phi) + B\cos(m\phi)$$

and

$$R = CJ_m(k\rho),$$

respectively ($J_m(k\rho)$ is the Bessel function of order m). According to our boundary condition, the wave function must vanish at $\rho = a$; k thus takes only special values,

$$k_{mn} = \frac{x_{mn}}{a}, \quad n = 1, 2, 3, \ldots, \tag{10.48}$$

where x_{mn} are the roots of the Bessel functions $J_m(x_{mn}) = 0$, listed in Table 5.2.

The general solution for a two-dimensional wave equation in polar coordinates is

$$\psi(\rho, \phi, t) = \sum_{m=0}^{\infty}\sum_{n=1}^{\infty} J_m(k_{mn}\rho)\cos(k_{mn}vt)[A_{mn}\sin(m\phi) + B_{mn}\cos(m\phi)]. \tag{10.49}$$

For each pair of m and n, this solution corresponds to a mode in two dimensions. Recall that a mode is a pattern of motion that oscillates at a fixed frequency: in one dimension it is characterized by only one index n, with frequency nkv; in two dimensions it is characterized by two indices m and n, with frequency $k_{mn}v$. Two-dimensional vibration can also be analyzed in various modes; it is a Fourier series in ϕ and a Fourier–Bessel series in ρ, for which the coefficients are evaluated from an initial condition $f(\rho, \theta)$,

$$A_{mn} = \frac{2}{\pi a^2 J_{m+1}^2(k_{mn}a)}\int_0^{2\pi} d\phi \int_0^a d\rho\rho f(\rho, \phi) J_m(k_{mn}\rho)\sin(m\phi), \tag{10.50}$$

and

$$B_{mn} = \frac{2}{\pi a^2 J_{m+1}^2(k_{mn}a)}\int_0^{2\pi} d\phi \int_0^a d\rho\rho f(\rho, \phi) J_m(k_{mn}\rho)\cos(m\phi). \tag{10.51}$$

All these calculations are identical to those encountered in relation to the theory of potential.

Example 10.6 A circular membrane of radius $a = 1$ is excited at $t = 0$ with an initial displacement

$$\psi(\rho, \phi, 0) = f(\rho, \phi) = \rho(a - \rho)\cos(2\phi).$$

Find the wave function $\psi(\rho, \phi, t)$ for $t > 0$.

Solution Because this initial condition contains $\cos(2\phi)$, the Fourier series is nonvanishing only for terms of B_{mn} with $m = 2$. We have

$$\int_0^{2\pi} [\cos(2\phi)]^2 d\phi = \pi;$$

we thus find B_{2n} as

$$B_{2n} = \frac{2}{a^2 J_3^2(k_{2n}a)} \int_0^a \rho[\rho(a-\rho)] J_2(k_{2n}\rho)\, d\rho.$$

The wave numbers are

$$k_{21} = \frac{x_{21}}{a} = 5.14, \quad k_{22} = \frac{x_{22}}{a} = 8.42, \quad k_{23} = \frac{x_{23}}{a} = 11.62, \quad k_{24} = \frac{x_{24}}{a} = 14.80, \ldots.$$

We have exploited an expansion of this type numerous times. The wave function is

$$\begin{aligned} \psi(\rho,\phi,t) &= 0.53 J_2(5.14\rho)\cos(2\phi)\cos(5.14vt) \\ &+ 0.098 J_2(8.42\rho)\cos(2\phi)\cos(8.42vt) \\ &+ 0.088 J_2(11.62\rho)\cos(2\phi)\cos(11.62vt) \\ &+ 0.034 J_2(14.80\rho)\cos(2\phi)\cos(14.80vt) \\ &+ \ldots. \end{aligned}$$

The frequencies of the first four modes are hence

$$\omega_{21} = k_{21}v = 5.14v, \quad \omega_{22} = k_{22}v = 8.42v, \quad \omega_{23} = k_{23}v = 11.62v, \quad \omega_{24} = k_{24}v = 14.80v, \ldots,$$

which are proportional to the roots of the Bessel functions listed in Table 5.2. Recall that for a one-dimensional vibrating string the frequencies are kv, $2kv$, $3kv$, ..., because the roots of sines occur at π, 2π, 3π, ... Unlike the situation of a one-dimensional vibration, the frequencies in a two-dimensional vibration are not simple multiples of each other; this lack of harmony provides an explanation as to why the sound from a percussion instrument, such as a drum, is cacophonous.

Worksheet 10.10 The procedure to calculate expansion coefficients is identical to that in Section 7.6. We produce an animation in three dimensions using the `animate` command.

```
> x2[1] := evalf(BesselJZeros(2,1));
                          x2[1] := 5.135622302
> x2[2] := evalf(BesselJZeros(2,2));
                          x2[2] := 8.417244140
> x2[3] := evalf(BesselJZeros(2,3));
                          x2[3] := 11.61984117
```

```
> x2[4] := evalf(BesselJZeros(2,4));
```

$$x2_4 := 14.79595178$$

```
> x2[5] := evalf(BesselJZeros(2,5));
```

$$x2_5 := 17.95981949$$

```
> a := 1; v :=1;
```

$$a := 1$$

$$v := 1$$

```
> N := 5:
> for n from 1 to N do
> k2[n] := x2[n]/a;
> end do:
> for n from 1 to N do
> B2[n] := 2/(a^2*BesselJ(3,k2[n]*a)^2)*int(rho*rho*(a-rho)
> *BesselJ(2,k2[n]*rho), rho=0..a);
> end do;
```

$$B2_1 := 0.5273837770$$

$$B2_2 := 0.09805457534$$

$$B2_3 := 0.08758732210$$

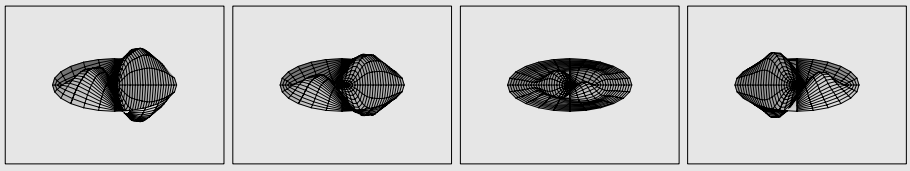
$$B2_4 := 0.03433336328$$

$$B2_5 := 0.03495744094$$

```
> psi :=  add(B2[n]*BesselJ(2,k2[n]*rho)*cos(2*phi)*cos(k2[n]*v*t),
> n=1..N);
```

$$\begin{aligned}\psi := {} & 0.5273837770\,\mathrm{BesselJ}(2,\,5.135622302\,\rho)\cos(2\,\phi)\cos(5.135622302\,t)\\ & + 0.09805457534\,\mathrm{BesselJ}(2,\,8.417244140\,\rho)\cos(2\,\phi)\cos(8.417244140\,t)\\ & + 0.08758732210\,\mathrm{BesselJ}(2,\,11.61984117\,\rho)\cos(2\,\phi)\cos(11.61984117\,t)\\ & + 0.03433336328\,\mathrm{BesselJ}(2,\,14.79595178\,\rho)\cos(2\,\phi)\cos(14.79595178\,t)\\ & + 0.03495744094\,\mathrm{BesselJ}(2,\,17.95981949\,\rho)\cos(2\,\phi)\cos(17.95981949\,t)\end{aligned}$$

```
> with(plots):
Warning, the name changecoords has been redefined
> animate(plot3d, [[rho*cos(phi), rho*sin(phi), psi], rho=0..a,
> phi=0..2*Pi], t=0..2*Pi/(v*k2[1]));
```



In the above example, we deliberately choose a problem for which expansion as a Fourier series only requires one particular m, but undertaking an expansion with many m terms is straightforward.

If the initial velocity is not zero, we must include an extra term in the temporal component:

$$T(t) = C\cos(k_{mn}vt) + D\sin(k_{mn}vt).$$

For this situation there is an exercise at the end of the chapter.

10.6 Electromagnetic Waves

We have studied electromagnetism in static conditions in Chapters 6, 7 and 8. The complete theory of electromagnetism is governed by the time-dependent Maxwell equations,

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \tag{10.52a}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{10.52b}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{10.52c}$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}. \tag{10.52d}$$

If there is no source, that is $\rho = 0$ and $\mathbf{J} = 0$, we can prove that these electric and magnetic fields conform to wave equations:

$$\nabla^2 \mathbf{E} = \mu_0 \epsilon_0 \frac{\partial^2 \mathbf{E}}{\partial t^2}, \tag{10.53}$$

and

$$\nabla^2 \mathbf{B} = \mu_0 \epsilon_0 \frac{\partial^2 \mathbf{B}}{\partial t^2}; \tag{10.54}$$

see an exercise at the end of this chapter. Each Cartesian component of the electric and magnetic fields satisfies the wave equation, in which the wave velocity is

$$v = \frac{1}{\sqrt{\mu_0 \epsilon_0}}. \tag{10.55}$$

Substituting in the values of permittivity and permeability of free space, we evaluate this velocity to be

$$v = 299\,792\,458 \text{ m s}^{-1},$$

which is precisely the speed of light c. This astonishing result provides strong evidence that light is an electromagnetic wave. One might be less impressed by this fact because the relation $c = \frac{1}{\sqrt{\epsilon_0 \mu_0}}$ is exact by definition in SI units, but the introduction of ϵ_0 and μ_0 is from experiments in electrostatics and magnetostatics: Coulomb's law in equation (6.1), and the Biot–Savart law in equation (8.9); the speed of light inevitably arises from the permittivity and permeability independent of the choice of units. We will discuss the interference of electromagnetic waves in Chapter 11; here we discuss the excitation of electromagnetic waves.

A general solution of the time-dependent Maxwell equations is found on first calculating the retarded scalar and vector potentials,

$$V(\mathbf{r}_1, t) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}_2, t_r)}{r_{12}} \, dV_2, \tag{10.56}$$

and

$$\mathbf{A}(\mathbf{r}_1, t) = \frac{\mu_0}{4\pi} \int \frac{\mathbf{J}(\mathbf{r}_2, t_r)}{r_{12}} \, dV_2, \tag{10.57}$$

respectively, where the retarded time is

$$t_r = t - \frac{r_{12}}{c}. \tag{10.58}$$

We denote $\mathbf{r}_1$ as the position vector for the field point, $\mathbf{r}_2$ as that for the source point, and $\mathbf{r}_{12}$ as the separation vector, just as defined in Section 6.1.

After we calculate the potentials, we obtain the electric field as

$$\mathbf{E} = -\nabla V - \frac{\partial \mathbf{A}}{\partial t}, \tag{10.59}$$

and magnetic field as

$$\mathbf{B} = \nabla \times \mathbf{A}. \tag{10.60}$$

We apply it to radiation from an electric dipole.

10.6.1 Electric-dipole Radiation

The most common method of generating an electromagnetic wave involves a dipole radiator, which is an electric dipole oscillating at frequency ω, see Figure 10.1, for which

$$q = q_0 \cos(\omega t). \tag{10.61}$$

The maximum magnitude of this dipole moment is

$$p = q_0 d.$$

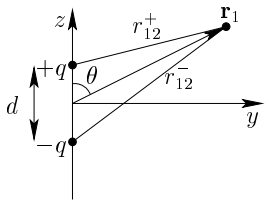


Figure 10.1: A radiating electric dipole.

We first calculate the scalar and vector potentials. For two point charges, the integral for the retarded scalar potential becomes a sum of two terms,

$$V(\mathbf{r}_1,t)=\frac{1}{4\pi\epsilon_0}\left\{\frac{q_0\cos[\omega(t-r_{12}^+/c)]}{r_{12}^+}+\frac{-q_0\cos[\omega(t-r_{12}^-/c)]}{r_{12}^-}\right\}, \tag{10.62}$$

where

$$r_{12}^{\pm}=\sqrt{r_1^2\mp r_1 d\cos\theta+(d/2)^2}. \tag{10.63}$$

Because the current is

$$\mathbf{I}(t)=\frac{dq}{dt}\hat{\mathbf{z}}=-q_0\sin(\omega t)\hat{\mathbf{z}}, \tag{10.64}$$

the retarded vector potential is

$$\mathbf{A}(\mathbf{r}_1,t)=\frac{\mu_0}{4\pi}\int_{-d/2}^{d/2}\frac{-q_0\omega\sin[\omega(t-r_{12}/c)]\hat{\mathbf{z}}}{r_{12}}dz, \tag{10.65}$$

where

$$r_{12}=\sqrt{r_1^2-r_1 z_2\cos\theta+(z_2/2)^2}. \tag{10.66}$$

In most situations we employ approximations to simplify the expressions, which we summarize as

$$d\ll\lambda\ll r_1. \tag{10.67}$$

Justifications of these approximations are that the physical size d of the electric dipole is much smaller than the wavelength, $\lambda=2\pi c/\omega$, and that an observer is located far from the dipole. We expand the scalar potential V as a function of d and retain only the linear d term. After such an expansion, we discard any term containing r to more negative powers than -1:

$$V=-\frac{p\omega}{4\pi\epsilon_0 c}\left(\frac{\cos\theta}{r_1}\right)\sin[\omega(t-r_1/c)]. \tag{10.68}$$

For the vector potential, because we make observations at a distance r, much larger than wavelength λ, we treat the integrand simply as a constant at $r_{12} \cong r_1$:

$$\mathbf{A} = -\frac{\mu_0 p\omega}{4\pi}\left(\frac{1}{r_1}\right)\sin[\omega(t - r_1/c)]\hat{\mathbf{z}}. \tag{10.69}$$

Hereafter we omit the subscript on r_1 for $V(\mathbf{r}_1, t)$ and $\mathbf{A}(\mathbf{r}_1, t)$, bearing in mind that r is the length of the position vector for the field point.

We proceed to evaluate the electric and magnetic fields. To calculate the curl and gradient of these vectors, spherical coordinates are convenient. We convert the vector potential from a Cartesian basis to a spherical basis, according to equation (6.18),

$$\hat{\mathbf{z}} = \cos\theta\,\hat{\mathbf{r}} - \sin\theta\,\hat{\boldsymbol{\theta}};$$

so

$$\mathbf{A} = -\frac{\mu_0 p\omega}{4\pi}\sin[\omega(t - r/c)]\left(\frac{\cos\theta}{r}\right)\hat{\mathbf{r}} + \frac{\mu_0 p\omega}{4\pi}\sin[\omega(t - r/c)]\left(\frac{\sin\theta}{r}\right)\hat{\boldsymbol{\theta}}. \tag{10.70}$$

The electric field is

$$\mathbf{E} = -\nabla V - \frac{\partial \mathbf{A}}{\partial t} = -\frac{\mu_0 p\omega^2}{4\pi}\left(\frac{\sin\theta}{r}\right)\cos[\omega(t - r/c)]\hat{\boldsymbol{\theta}}, \tag{10.71}$$

and the magnetic field is

$$\mathbf{B} = \nabla \times \mathbf{A} = -\frac{\mu_0 p\omega^2}{4\pi c}\left(\frac{\sin\theta}{r}\right)\cos[\omega(t - r/c)]\hat{\boldsymbol{\phi}}; \tag{10.72}$$

in both equations we discard any term containing r^{-1} to more negative powers than -1.

The energy radiated from an oscillating electric dipole is determined by the Poynting vector,

$$\mathbf{S} = \frac{1}{\mu_0}(\mathbf{E} \times \mathbf{B}) = \frac{\mu_0}{c}\frac{p^2\omega^4}{(4\pi)^2}\left(\frac{\sin\theta}{r}\right)^2\cos^2[\omega(t - r/c)]\hat{\mathbf{r}}. \tag{10.73}$$

Worksheet 10.11 The formalism is straightforward; the complicated approximations, which involve only the Taylor expansion, are readily performed by the `taylor` command. To calculate the gradient and curl in spherical coordinates, we employ the `Gradient` and `Curl` commands in the `VectorCalculus` package, with an appropriate setting of the `SetCoordinates` option.

```
> with(LinearAlgebra): with(VectorCalculus):
Warning, the names CrossProduct and DotProduct have been rebound
Warning, the assigned names <,> and <|> now have a global binding
```

```
Warning, these protected names have been redefined and unprotected: *,
+, ., Vector, diff, int, limit, series
> assume(r>0);
> V1 := 1/(4*Pi*epsilon[0])*(q*cos(omega*(t - rp/c))/rp -
> q*cos(omega*(t - rm/c))/rm);
```

$$V1 := \frac{1}{4}\,\frac{\dfrac{q\cos\left(\omega\,\left(t-\dfrac{rp}{c}\right)\right)}{rp}-\dfrac{q\cos\left(\omega\,\left(t-\dfrac{rm}{c}\right)\right)}{rm}}{\pi\,\varepsilon_0}$$

```
> rp := sqrt(r^2 - r*d*cos(theta) + (d/2)^2);
```

$$rp := \frac{1}{2}\,\sqrt{4\,r^2-4\,r\,d\cos(\theta)+d^2}$$

```
> rm := sqrt(r^2 + r*d*cos(theta) + (d/2)^2);
```

$$rm := \frac{1}{2}\,\sqrt{4\,r^2+4\,r\,d\cos(\theta)+d^2}$$

```
> V1:
> V1 := convert(taylor(V1, d=0, 2), polynom);
```

$$V1 := \frac{1}{4}\,\frac{\left(\dfrac{q\cos\left(\omega\,\left(t-\dfrac{r}{c}\right)\right)\,\cos(\theta)}{r^2}-\dfrac{q\sin\left(\omega\,\left(t-\dfrac{r}{c}\right)\right)\,\omega\cos(\theta)}{c\,r}\right)\,d}{\pi\,\varepsilon_0}$$

```
> V1 := subs({1/r^2=0}, V1);
```

$$V1 := -\frac{1}{4}\,\frac{q\sin\left(\omega\,\left(t-\dfrac{r}{c}\right)\right)\,\omega\cos(\theta)\,d}{\pi\,\varepsilon_0\,c\,r}$$

```
> V1 := algsubs(q*d=p, V1);
```

$$V1 := -\frac{1}{4}\,\frac{\sin\left(\omega\,\left(t-\dfrac{r}{c}\right)\right)\,\omega\cos(\theta)\,p}{\pi\,\varepsilon_0\,c\,r}$$

```
> Current := -q*omega*sin(omega*t);
```

$$Current := -q\,\omega\sin(\omega\,t)$$

```
> Az := mu[0]/(4*Pi)*subs(t=t-r/c, Current)*d/r;
```

$$Az := -\frac{1}{4}\,\frac{\mu_0\,q\,\omega\sin\left(\omega\,\left(t-\dfrac{r}{c}\right)\right)\,d}{\pi\,r}$$

```
> Az := algsubs(q*d=p, Az);
```

$$Az := -\frac{1}{4}\,\frac{\mu_0\,\omega\sin\left(\omega\,\left(t-\dfrac{r}{c}\right)\right)\,p}{\pi\,r}$$

```
> SetCoordinates('spherical'[r, theta, phi]);
```

$$spherical_{r,\,\theta,\,\phi}$$

```
> Avec := VectorField(<Az*cos(theta), -Az*sin(theta), 0>);
```

$$Avec := -\frac{1}{4}\frac{\mu_0\,\omega\sin\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,p\cos(\theta)}{\pi\,r}\bar{\mathbf{e}}_{\mathbf{r}}+\frac{1}{4}\frac{\mu_0\,\omega\sin\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,p\sin(\theta)}{\pi\,r}\bar{\mathbf{e}}_{\boldsymbol{\theta}}$$

```
> Epr11 := Gradient(V1);
```

$$Epr11 := \left(\frac{1}{4}\frac{\cos\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,\omega^2\cos(\theta)\,p}{\pi\,\varepsilon_0\,c^2\,r}+\frac{1}{4}\frac{\sin\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,\omega\cos(\theta)\,p}{\pi\,\varepsilon_0\,c\,r^2}\right)\bar{\mathbf{e}}_{\mathbf{r}}$$

$$+\frac{1}{4}\frac{\sin\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,\omega\sin(\theta)\,p}{r^2\,\pi\,\varepsilon_0\,c}\bar{\mathbf{e}}_{\boldsymbol{\theta}}$$

```
> Epr12 := map(curry(subs, 1/r^2=0), Epr11);
```

$$Epr12 := \frac{1}{4}\frac{\cos\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,\omega^2\cos(\theta)\,p}{\pi\,\varepsilon_0\,c^2\,r}\bar{\mathbf{e}}_{\mathbf{r}}$$

```
> Epr13 := map(diff, Avec, t);
```

$$Epr13 := -\frac{1}{4}\frac{\mu_0\,\omega^2\cos\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,p\cos(\theta)}{\pi\,r}\bar{\mathbf{e}}_{\mathbf{r}}+\frac{1}{4}\frac{\mu_0\,\omega^2\cos\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,p\sin(\theta)}{\pi\,r}\bar{\mathbf{e}}_{\boldsymbol{\theta}}$$

```
> epsilon[0] := 1/(mu[0]*c^2);
```

$$\varepsilon_0 := \frac{1}{\mu_0\,c^2}$$

```
> Efield := -Epr12 - Epr13;
```

$$Efield := -\frac{1}{4}\frac{\mu_0\,\omega^2\cos(\omega\,(t-\frac{r}{c}))\,p\sin(\theta)}{\pi\,r}\bar{\mathbf{e}}_{\boldsymbol{\theta}}$$

```
> Epr21 := Curl(Avec);
```

$$Epr21 := \frac{-\frac{1}{4}\frac{\mu_0\,\omega^2\cos\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,p\sin(\theta)}{\pi\,c}-\frac{1}{4}\frac{\mu_0\,\omega\sin\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,p\sin(\theta)}{\pi\,r}}{r}\bar{\mathbf{e}}_{\boldsymbol{\phi}}$$

```
> Epr22 := map(collect, Epr21, r);
```

$$Epr22 := \left(-\frac{1}{4}\frac{\mu_0\,\omega^2\cos\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,p\sin(\theta)}{\pi\,c\,r}-\frac{1}{4}\frac{\mu_0\,\omega\sin\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,p\sin(\theta)}{\pi\,r^2}\right)\bar{\mathbf{e}}_{\boldsymbol{\phi}}$$

```
> Bfield := map(curry(subs, 1/r^2=0), Epr22);
```

$$Bfield := -\frac{1}{4}\frac{\mu_0\,\omega^2\cos\left(\omega\,\left(t-\frac{r}{c}\right)\right)\,p\sin(\theta)}{\pi\,c\,r}\bar{\mathbf{e}}_{\boldsymbol{\phi}}$$

```
> Poynting := ScalarMultiply(CrossProduct(Efield, Bfield),
1/mu[0]):
> Poynting := map(simplify, Poynting);
```

$$Poynting := \begin{bmatrix} -\frac{1}{16}\,\dfrac{\mu_0\,\omega^4\cos\left(\dfrac{\omega\,(t\,c-r)}{c}\right)^2 p^2\,(-1+\cos(\theta)^2)}{r^2\,\pi^2\,c} \\ 0 \\ 0 \end{bmatrix}$$

To average an oscillating system over a complete cycle, we perform an integration:

$$\frac{1}{T}\int_0^T \cos^2[\omega(t-r/c)]dt = \frac{1}{2}, \quad \left(T = \frac{2\pi}{\omega}\right).$$

Therefore, the mean of the Poynting vector is

$$\overline{\mathbf{S}} = \frac{\mu_0 p^2 \omega^4}{32\pi^2 c}\left(\frac{\sin\theta}{r}\right)^2 \hat{\mathbf{r}}. \tag{10.74}$$

The Poynting vector signifies the energy per unit time per unit area transported by the fields. To find the total power radiated, we integrate over a sphere of radius r:

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \frac{\sin^2\theta}{r^2} r^2 \sin\theta = \frac{8\pi}{3}.$$

The power radiated by an electric dipole is therefore

$$\overline{P} = \int \overline{\mathbf{S}} \cdot d\mathbf{a} = \frac{\mu_0 p^2 \omega^4}{12\pi c}. \tag{10.75}$$

The Poynting vector contains a term $\sin^2\theta$, which gives the angular distribution of the power of radiation; we plot such a pattern in the following worksheet.

Worksheet 10.12 Maple can readily evaluate these basic integrals, and plot the angular distribution of the power.

```
> T := 2*Pi/omega;
```

$$T := \frac{2\,\pi}{\omega}$$

```
> Epr1 := cos(omega*(t-r/c));
```

$$Epr1 := \cos\left(\omega\,\left(t-\frac{r}{c}\right)\right)$$

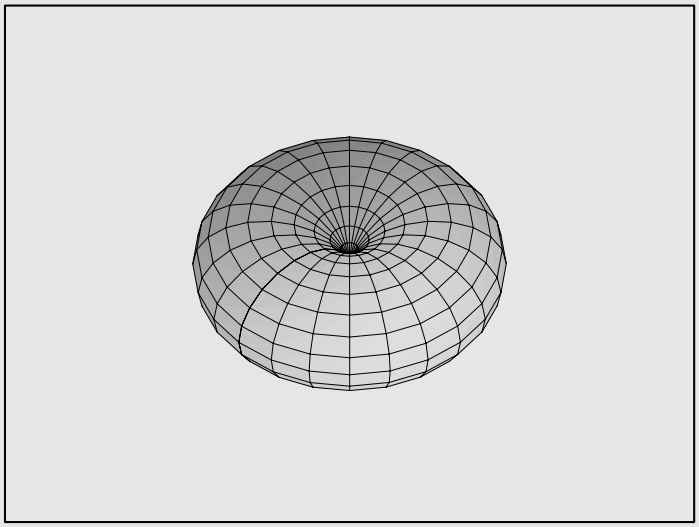
```
> Epr2 := 1/T*int(Epr1^2, t=0..T);
```

$$Epr2 := \frac{1}{2}$$

```
> Epr3 := 2*Pi*int(sin(theta)^2/r^2*r^2*sin(theta), theta=0..Pi);
```

$$Epr3 := \frac{8\,\pi}{3}$$

```
> plots[sphereplot](sin(theta)^2, phi=0..2*Pi, theta=0..Pi,
> scaling=constrained);
```



From the plot, we notice that no radiation is emitted along the axis of the dipole.

10.6.2 Synchrotron Radiation

Synchrotron radiation refers to the radiation emitted by a charged particle moving at nearly the speed of light along a circular path (instantaneously); the acceleration for the circular motion is provided by a Lorentz force ($e\mathbf{v} \times \mathbf{B}$) in a magnetic field. This phenomenon is observed in many astronomical systems; it is also utilized as a powerful tool for the investigation of the optical properties of solids. This subject is complicated and knowledge of special relativity is required. In this section, we adopt equations from Jackson's *Classical Electrodynamics* without derivation, and use Maple to illustrate important features of the angular and spectral distribution of synchrotron radiation.

In relativity, two of the most important definitions are

$$\beta = \frac{v}{c}, \quad \gamma = \frac{1}{\sqrt{1-\beta^2}}, \tag{10.76}$$

see Chapter 12 for an additional discussion. A high-speed electron in the presence of a magnetic field undergoes circular motion, and the rate of energy loss P is proportional to γ to the

fourth power, or more precisely[2]

$$P = \frac{e^2 c}{6\pi\epsilon_0 R^2}\gamma^4, \tag{10.77}$$

where R is the radius of circular orbit. The angular distribution of power is[3]

$$\frac{dP}{d\Omega} = \frac{e^2 c}{16\pi^2\epsilon_0 R^2}\frac{1}{(1-\beta\cos\theta)^3}\left[1 - \frac{\sin^2\theta\cos^2\phi}{\gamma^2(1-\beta\cos\theta)^2}\right]; \tag{10.78}$$

integrating this formula over all angles gives equation (10.77), which we leave as an exercise. We plot the angular distribution below.

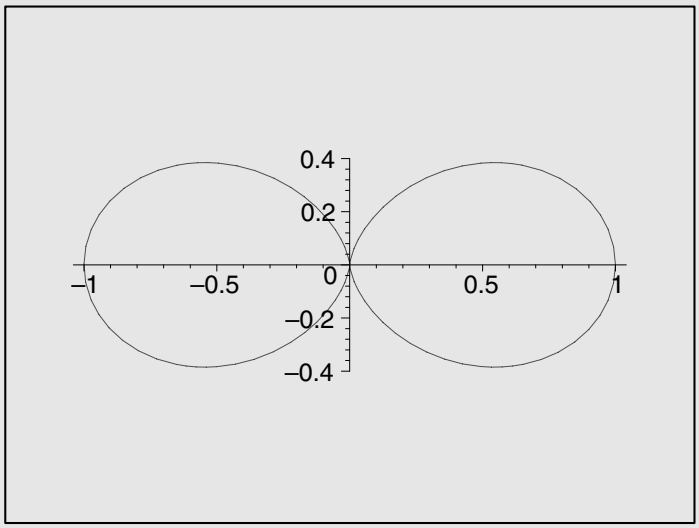
Worksheet 10.13 In this worksheet, we define that the charged particle moves in the x direction (horizontal axis), while the acceleration is in the z direction (vertical axis); θ is measured with respect to the x axis.

```
> beta := 0; g := 1/sqrt(1 - beta^2);
```

$$\beta := 0$$

$$g := 1$$

```
> plot(1/(1 - beta*cos(theta))^3*(1 - sin(theta)^2/(g*(1 -
> beta*cos(theta)))^2), theta=0..2*Pi, coords=polar,
> scaling=constrained);
```



[2]Jackson 1999, equation (14.31), p. 667, or Griffiths 1999, problem 11.16, p. 465. Note that the acceleration for circular motion is v^2/r; we replace a in the latter reference with c^2/R because the particle moves at essentially the speed of light and the radius of a synchrotron radiation facility is fixed.

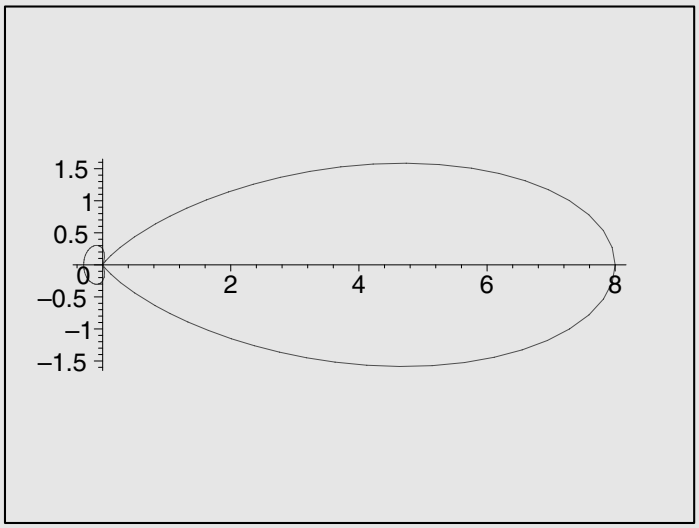
[3]Jackson 1999, equation (14.44), p. 670, or Griffiths ibid.

```
> beta := 0.5; g := 1/sqrt(1 - beta^2);
```

$$\beta := 0.5$$

$$g := 1.154700538$$

```
> plot(1/(1 - beta*cos(theta))^3*(1 - sin(theta)^2/(g*(1 -
> beta*cos(theta)))^2), theta=0..2*Pi, coords=polar,
> scaling=constrained);
```



For $\beta = 0$, the angular distribution is identical to that of the electric-dipole radiation seen in the preceding worksheet. When β is $1/2$, implying half the speed of light, the radiation is sharply peaked in the forward direction. Increasing the velocity makes it tip forward more, and with a larger magnitude, which we leave the reader to discover by modifying the worksheet. This plot illustrates the "searchlight" pattern of synchrotron radiation; the peaking is concentrated within $\theta \lesssim 1/\gamma$.

Because emitted radiation is confined within a narrow cone in the direction of the velocity vector, it sweeps past an observer in a time interval much smaller than the period for an electron to make one revolution; in other words, only a short pulse of radiation is detected. Based on the uncertainty principle, a short pulse must be made of a broad range of frequencies. The precise formula for the spectral distribution of synchrotron radiation is complicated, which involves the modified Bessel function $K_\nu(x)$. Nevertheless, Maple supports this function, named `BesselK(nu, x)`. Defining a critical frequency[4]

$$\omega_c \equiv \frac{3\gamma^3 c}{2R}, \tag{10.79}$$

[4]Jackson 1999, equation (14.81), p. 679.

the energy radiated per unit frequency interval is[5]

$$\frac{dI}{d\omega} = \sqrt{3}\frac{e^2}{4\pi\epsilon_0 c}\gamma\frac{\omega}{\omega_c}\int_{\omega/\omega_c}^{\infty} K_{5/3}(x)\,dx. \tag{10.80}$$

For a periodic circular motion, the spectrum is actually discrete, consisting of frequencies that are integer multiples of the fundamental frequency $\omega_0 = c/R$. The power radiated into the nth multiple of ω_0 is[6]

$$P_n = \frac{1}{2\pi}\left(\frac{c}{R}\right)^2 \left.\frac{dI}{d\omega}\right|_{\omega=n\omega_0}. \tag{10.81}$$

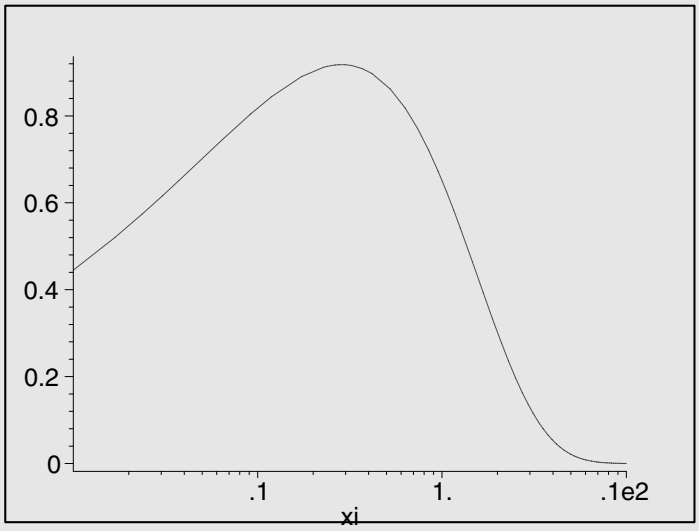
The spectral dependence is determined by this part:

$$F(\xi) \equiv \xi\int_{\xi}^{\infty} K_{5/3}(x)\,dx, \tag{10.82}$$

where $\xi \equiv \omega/\omega_c$. This integral certainly looks difficult, but Maple can perform it, and produce a plot, which illustrates the pattern of the spectrum of synchrotron radiation, while the frequency is expressed in units of ω_c (equation (10.79)).

Worksheet 10.14 Because the spectral distribution extends over a broad range, the `semilogplot` command serves to impose a logarithmic scale on the horizontal axis. The reader can render a plot on a linear scale.

```
> F := xi*int(BesselK(5/3, x), x=xi..infinity):
> plots[semilogplot](F, xi=0.01..10, axes=frame);
```



[5] Jackson 1999, equation (14.91), p. 681.
[6] Jackson 1999, equation (14.92), p. 681.

This plot shows that synchrotron radiation spread over a broad frequency distribution – the uncertainty principle $\Delta\omega\,\Delta t \gtrsim 1/2$ is at work again. The peak occurs at $\omega = 0.2858\,\omega_c$, which we leave as an exercise. In practice, synchrotron covers the visible, ultraviolet to X-ray regions. Several synchrotron light facilities exist as derivative installations attached to storage rings of high-energy experiments, but in recent years synchrotron radiation facilities have been built exclusively to generate a high-quality light source to enable condensed-matter physicists and biologists to conduct research. For example, the Advanced Light Source of the Berkeley Lab has a circumference of 196.8 m and a nominal energy of 1.9 GeV;[7] from these data we obtain $\gamma \simeq 3718$ (1.9 GeV divided by the rest mass of the electron 0.511 MeV, see equation (12.31)) and $R \simeq 31.3$ m (the path is not exactly circular). The fundamental frequency is $\omega_0 = c/R \simeq 9.57$ MHz, but the peak is at $0.2858\,\omega_c \simeq 2.11 \times 10^{17}$ Hz, which corresponds to X-rays of 0.87 keV.

Exercises

1. A string of length $l = 3$ is disturbed by an initial displacement

$$f(x) = \begin{cases} x, & 0 < x < 1, \\ \dfrac{3}{2} - \dfrac{x}{2}, & 1 < x < 3, \end{cases}$$

and an initial velocity

$$g(x) = x(x-3), \quad 0 < x < 3.$$

Derive the wave equation $\psi(x,t)$ for $t > 0$.
Hint: in addition to a_n, we must evaluate b_n in equation (10.15) for the series $\sin(nkvt)$.

2. A circular membrane similar to that in Section 10.5 is subject to an initial condition

$$\psi(\rho,\phi,0) = f(\rho,\phi) = \cos\Big(\frac{\pi\rho}{2}\Big)\sin\phi.$$

Calculate the wave function $\psi(\rho,\phi,t)$.

For the same initial displacement, find an expression for the wave function if additionally it is released with initial velocity

$$\left.\frac{\partial\psi}{\partial t}\right|_{t=0} = g(\rho,\phi) = (\rho-1)\,\cos\left(\frac{\pi\phi}{2}\right),$$

for which one must consider also terms in $\sin t$.

[7] See `http://www-als.lbl.gov` for more information.

3. (a) Employing the `VectorCalculus` package, verify by a direct calculation that

$$\nabla \times (\nabla \times \mathbf{a}) = \nabla(\nabla \cdot \mathbf{a}) - \nabla^2 \mathbf{a}, \tag{10.83}$$

where $\mathbf{a}$ is an arbitrary vector field.

(b) Apply the curl to equations (10.52b) and (10.52d), verify that Maxwell's equations in a region of space free of charge and current become the wave equations.

4. Verify that the total power radiated by an oscillating magnetic dipole $\mathbf{m}(t) = m_0 \cos(\omega t)\hat{\mathbf{z}}$ is

$$\overline{P} = \frac{\mu_0 m_0^2 \omega^4}{12\pi c^3}. \tag{10.84}$$

Hint: consult Griffiths 1999, p. 451.

5. Based on a crude model, an atom can be treated as an oscillator in which an electron is driven up and down by an electromagnetic field, and such an electron is subject to a linear restoring force.

(a) The differential equation governing such a system is

$$m\ddot{x} + m\omega_0^2 x = eE_0 \cos(\omega t); \tag{10.85}$$

show that the steady-state solution is

$$x = \frac{eE_0}{m(\omega_0^2 - \omega^2)} \cos(\omega t). \tag{10.86}$$

(b) Using equation (10.75), show that the power of radiation emitted by such an oscillator is

$$\overline{P} = \frac{e^2 \omega^4}{12\pi\epsilon_0 c^3} \left[\frac{eE_0}{m(\omega_0^2 - \omega^2)}\right]^2. \tag{10.87}$$

(c) The intensity of an incident wave is

$$\overline{I} = \frac{1}{2}\epsilon_0 c E_0^2, \tag{10.88}$$

and the scattering cross-section is defined as

$$\sigma = \frac{\overline{P}}{\overline{I}}, \tag{10.89}$$

show that

$$\sigma = \frac{8\pi r_e^2}{3} \frac{\omega^4}{(\omega^2 - \omega_0^2)^2}, \quad r_e \equiv \frac{e^2}{4\pi\epsilon_0 m c^2}, \tag{10.90}$$

where r_e is the classical radius of the electron. When ω is small compared with ω_0, we can disregard ω^2 in the denominator, and the power of radiation is proportional to the *fourth* power of the frequency. This process is called Rayleigh scattering; it is responsible for the blue color of the sky because it favors the scattering of light of higher frequency. In an extreme when ω_0 is zero, which corresponds to a free electron, we obtain the cross-section of Thomson scattering as introduced in an exercise in Chapter 2.

6. (a) Integrate the angular distribution of synchrotron radiation over all angles, that is

$$\int \frac{dP}{d\Omega} d\Omega = \frac{e^2 c}{16\pi^2 \epsilon_0 R^2} \int_0^{\pi} d\theta \int_0^{2\pi} d\phi \, \frac{1}{(1-\beta\cos\theta)^3} \left[1 - \frac{\sin^2\theta\cos^2\phi}{\gamma^2(1-\beta\cos\theta)^2}\right] \sin\theta, \tag{10.91}$$

to verify the formula of total power in equation (10.77).

(b) To find the frequency at which the power of synchrotron radiation reaches a maximum, one needs to find the root to the equation

$$\frac{dF(\xi)}{d\xi} = 0,$$

where $F(\xi)$ is defined in equation (10.82). Verify that the root is $\xi = 0.2858$.

7. In synchrotron radiation, the charged particle undergoes circular motion, thus acceleration is perpendicular to velocity. In a linear motion in which acceleration and velocity are parallel, the angular distribution is[8]

$$\frac{dP}{d\Omega} = \frac{e^2 a^2}{16\pi^2 \epsilon_0 c^3} \frac{\sin^2\theta}{(1-\beta\cos\theta)^5}. \tag{10.92}$$

(a) Plot the angular distribution for $\beta \simeq 0$ and $\beta \lesssim 1$, which should resemble Figure 10.2. Although this angular distribution is different from that of synchrotron radiation, a similar characteristic relativistic peaking at forward angles is present. Generation of X-rays through "bremsstrahlung," or braking radiation, conforms with this pattern based on classical theory.

(b) Verify that the total power is

$$P = \frac{e^2 a^2 \gamma^6}{6\pi\epsilon_0 c^3}, \tag{10.93}$$

by performing an integral

$$P = \int \frac{dP}{d\Omega} d\Omega = \frac{e^2 a^2}{16\pi^2 \epsilon_0 c^3} \int_0^{\pi} d\theta \int_0^{2\pi} d\phi \, \frac{\sin^2\theta}{(1-\beta\cos\theta)^5} \sin\theta. \tag{10.94}$$

[8] Jackson 1999, equation (14.39), p. 669, or Griffiths 1999, equation (11.74), p. 463.

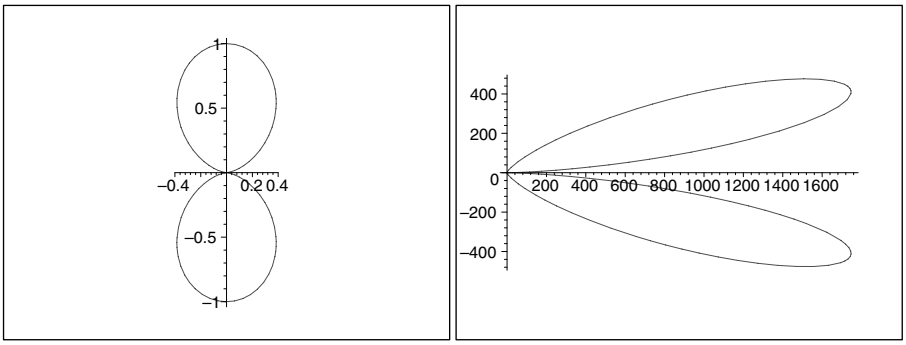


Figure 10.2: Radiation pattern for $\beta = 0$ and $\beta = 0.9$.

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11 Physical Optics

From the calculated speed of electromagnetic waves, Maxwell argued that light must be an electromagnetic wave. Physical optics is a manifestation of the wave nature of light, and the mathematics involved in its treatment simply involves the addition of waves. Maple can perform this task by directly adding waves graphically, as well as by deriving algebraic formulas.

11.1 Light as an Electromagnetic Wave

Electric and magnetic fields in a space free of charge and current satisfy these equations:

$$\nabla^2 \mathbf{E} = \mu_0 \epsilon_0 \frac{\partial^2 \mathbf{E}}{\partial t^2}, \tag{11.1}$$

$$\nabla^2 \mathbf{B} = \mu_0 \epsilon_0 \frac{\partial^2 \mathbf{B}}{\partial t^2}. \tag{11.2}$$

Each Cartesian component of the electric field $\mathbf{E}$ and the magnetic field $\mathbf{B}$ therefore satisfies a wave equation,

$$\nabla^2 \psi = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2}, \tag{11.3}$$

where ψ is one component of either field, such as E_x or B_y. As stated in the preceding chapter, the speed of an electromagnetic wave is

$$v = \frac{1}{\sqrt{\mu_0 \epsilon_0}} = 299\,792\,458 \text{ m s}^{-1}, \tag{11.4}$$

which is by definition the speed of light in a vacuum. An implication of this result is that light is an electromagnetic wave, as Maxwell deduced.

For most of this chapter, our interest lies in monochromatic plane waves, such that waves of a single frequency travel in the x direction. The fields describing such a wave are

$$\mathbf{E} = \mathbf{E}_0 \cos(kx - \omega t + \varphi), \quad \mathbf{B} = \mathbf{B}_0 \cos(kx - \omega t + \varphi). \tag{11.5}$$

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ISBN: 3-527-40640-9

Electromagnetic waves are transverse waves: their oscillation is perpendicular to the direction of propagation. Therefore,

$$\mathbf{E}_0 \cdot \hat{\mathbf{x}} = 0, \quad \mathbf{B}_0 \cdot \hat{\mathbf{x}} = 0. \tag{11.6}$$

From these results we understand that $\mathbf{E}_0$ and $\mathbf{B}_0$ possess only y and z components. Because the effect of magnetic field is generally small, from this point onward we discuss electric field only.

11.1.1 Polarization

We express an electromagnetic wave in complex notation as

$$\mathbf{E} = \Re\left\{\tilde{\mathbf{E}}_0 e^{i(kx-\omega t)}\right\}, \tag{11.7}$$

where $\tilde{\mathbf{E}}_0$ is complex because it contains information about the phase angle; see the discussion in Section 10.3.1.

The electric vector $\tilde{\mathbf{E}_0}$ expresses the polarization of the wave. Because this vector is perpendicular to x, we can construct it from two independent states of polarization in the y and z directions,

$$\tilde{\mathbf{E}}_0 = \tilde{E}_{0y}\hat{\mathbf{y}} + \tilde{E}_{0z}\hat{\mathbf{z}}. \tag{11.8}$$

Generally $\tilde{E}_{0y}$ and $\tilde{E}_{0z}$ are also complex; they can be expressed in polar form as

$$\tilde{E}_{0y} = E_{0y}e^{i\alpha_y}, \quad \tilde{E}_{0z} = E_{0z}e^{i\alpha_z},$$

where E_{0y} and E_{0z} are the magnitudes of the maximum amplitude in the corresponding directions. Note that α_y and α_z need not be equal to each other.

We write the field as

$$\mathbf{E} = E_{0y}\cos(kx - \omega t + \varphi + \alpha_y)\hat{\mathbf{y}} + E_{0z}\cos(kx - \omega t + \varphi + \alpha_z)\hat{\mathbf{z}}. \tag{11.9}$$

This equation indicates that y and z components of electric field oscillate at the same frequency, but not necessarily with the same phase. The polarization of a wave is characterized by the magnitudes E_{0y} and E_{0z} and by the phase difference between α_y and α_z.

If $\alpha_y = \alpha_z$, there is no phase difference; the wave is described as being linearly polarized, or plane polarized.

If $\alpha_y \neq \alpha_z$, there is a phase difference; the wave is described as being elliptically polarized. The reason for this term is that, for fixed x, the tip of the electric field vector rotates in a plane parallel to the yz plane; the trajectory of the arrowhead of this vector is an ellipse. When $E_{0y} = E_{0z}$ and $|\alpha_y - \alpha_z| = \pi/2$, the ellipse becomes a circle; the wave is described as being circularly polarized.

We fix time and plot the electric vector in various polarizations. The projection of such a plot in a plane parallel to the yz plane is a line, an ellipse, or a circle, depending on E_{0y}, E_{0z}, and $\alpha_y - \alpha_z$. The projection on the xy or xz plane is a sinusoidal curve, with corresponding phase angle.

With Maple we produce graphs for various polarizations.

Worksheet 11.1 We plot the projection on the yz and xz planes, and a view in three dimensions using the `spacecurve` command. To observe the variation, alter the values of E_{0y}, E_{0z}, and $\alpha_z - \alpha_y$, which we denote as `beta` in this worksheet.

```
> E0y := 5; E0z :=5; beta := Pi/4; k := 2;
```

$$E0y := 5$$
$$E0z := 5$$
$$\beta := \frac{\pi}{4}$$
$$k := 2$$

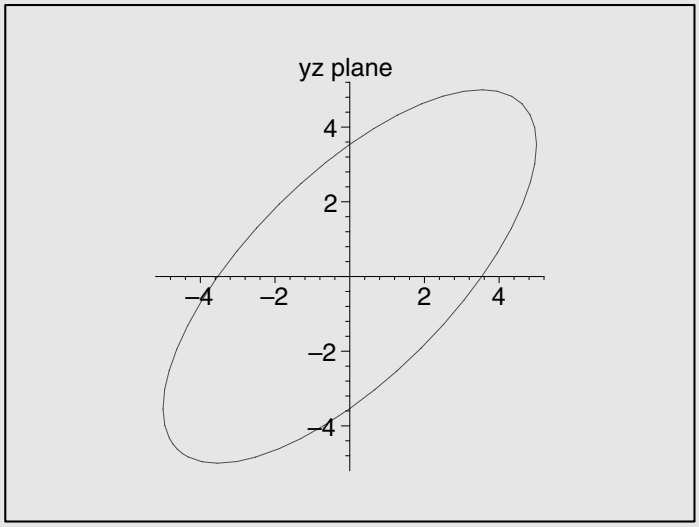
```
> Ey := E0y*cos(k*x);
```

$$Ey := 5\cos(2\,x)$$

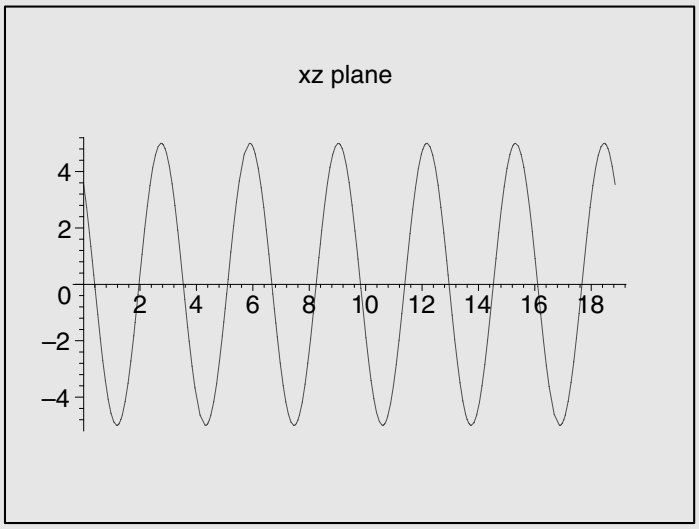
```
> Ez := E0z*cos(k*x + beta);
```

$$Ez := 5\cos(2\,x + \frac{\pi}{4})$$

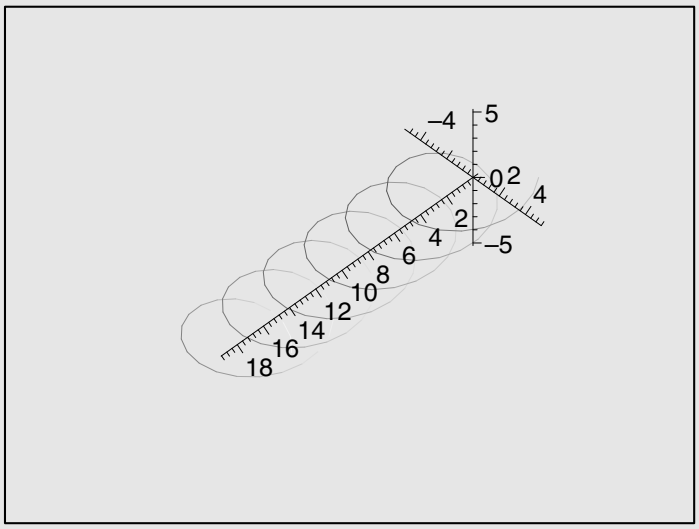
```
> plot([Ey, Ez, x=0..2*Pi/k], scaling=constrained,
> title="yz plane");
```




```
> plot([x, Ez, x=0..6*2*Pi/k], scaling=constrained,
> title="xz plane");
```




```
> with(plots):
Warning, the name changecoords has been redefined
> spacecurve([x, Ey, Ez, x=0..6*2*Pi/k], thickness=2,
> numpoints=120, scaling=constrained, axes=normal);
```



An elliptical polarization is shown in the worksheet. By varying the numerical values of E_x, E_y, and their phase difference β, one can visualize different polarizations, which we leave as an exercise.

11.2 Mathematics of Interference

Mathematically, the interference of waves involves finding the sum ψ of two waves of the same frequency but different phase:

$$\psi = \psi_1 + \psi_2 = A_1 \cos(\omega t + \varphi_1) + A_2 \cos(\omega t + \varphi_2). \tag{11.10}$$

The combination of two waves naturally retains the same frequency; we need to find the amplitude and phase for the composite wave ψ.

We mention in Section 10.3.1 that complex notation is convenient to represent waves, because it is easier to manipulate exponentials than sines and cosines; consult that section for an explanation of the notation. We write ψ as

$$\psi = \Re\left\{A_1 e^{i(\omega t+\varphi_1)} + A_2 e^{i(\omega t+\varphi_2)}\right\}.$$

Defining

$$\tilde{\psi} = \tilde{A}_t e^{i\omega t}, \quad \tilde{\psi}_1 = \tilde{A}_1 e^{i\omega t}, \quad \tilde{\psi}_2 = \tilde{A}_1 e^{i\omega t},$$

where complex amplitudes are

$$\tilde{A}_t = A_t e^{i\varphi_t}, \quad \tilde{A}_1 = A_1 e^{i\varphi_1}, \quad \tilde{A}_2 = A_2 e^{i\varphi_2},$$

we have

$$\tilde{\psi} = \tilde{\psi}_1 + \tilde{\psi}_2, \quad \psi = \Re\{\tilde{\psi}\}.$$

Eliminating a common factor $e^{i\omega t}$ yields

$$\tilde{A}_t = \tilde{A}_1 + \tilde{A}_2, \quad \text{or} \quad A_t e^{i\varphi_t} = A_1 e^{i\varphi_1} + A_2 e^{i\varphi_2}.$$

We readily find the magnitude of the amplitude A_t as the complex scalar product of $\tilde{A}_t$,

$$A_t^2 = \tilde{A}_t \tilde{A}_t^* = A_1^2 + A_2^2 + 2A_1 A_2 \cos(\varphi_2 - \varphi_1). \tag{11.11}$$

Worksheet 11.2 The complex scalar product is a complex number multiplied by its complex conjugate. To form the conjugate of a complex number, Maple provides a command `conjugate`. We employ the `evalc` command to simplify a complex expression. The `combine` command is useful to further simplify a trigonometric expression.

```
> At := A1*exp(I*phi1) + A2*exp(I*phi2);
```

$$At := A1\, e^{(\phi 1\, I)} + A2\, e^{(\phi 2\, I)}$$

```
> Epr1 := At*conjugate(At);
```

$$Epr1 := (A1\, e^{(\phi 1\, I)} + A2\, e^{(\phi 2\, I)})\, \overline{(A1\, e^{(\phi 1\, I)} + A2\, e^{(\phi 2\, I)})}$$

```
> Epr2 := evalc(Epr1):
> Epr3 := simplify(Epr2):
> Epr4 := combine(Epr3);
```

$$Epr4 := 2\, A1\, A2 \cos(\phi 1 - \phi 2) + A1^2 + A2^2$$

We can extend the technique of adding two waves to adding multiple waves. Suppose that we have n waves, all of equal amplitude but differing in phase φ; we seek the sum of

$$\psi = A[\cos(\omega t) + \cos(\omega t + \varphi) + \cos(\omega t + 2\varphi) + \ldots + \cos(\omega t + (n-1)\varphi)]. \quad (11.12)$$

In principle, we can find the final amplitude using a graphical method. Here is an illustrative example.

Example 11.1 Five wave sources have the same frequency but successive differences in phase by $\pi/10$. Find the amplitude of the composite wave.

Solution In this problem, we have $n = 5$ and $\varphi = \pi/10$. We form a plot of these waves and their combination in a fixed position. The amplitude of the composite, which is the maximum, is $4.52A$.

Worksheet 11.3 Maple can conveniently produce plots of combination of waves; to find the resultant amplitude we use the `maximize` command. One can vary ϕ to observe the effect of the phase angle on the amplitude of the composite.

```
> psi[1] := cos(t);
```

$$\psi_1 := \cos(t)$$

```
> psi[2] := cos(t+phi);
```

$$\psi_2 := \cos(t + \phi)$$

```
> psi[3] := cos(t+2*phi);
```

$$\psi_3 := \cos(t + 2\,\phi)$$

```
> psi[4] := cos(t+3*phi);
```

$$\psi_4 := \cos(t + 3\,\phi)$$

```
> psi[5] := cos(t+4*phi);
```

$$\psi_5 := \cos(t + 4\,\phi)$$

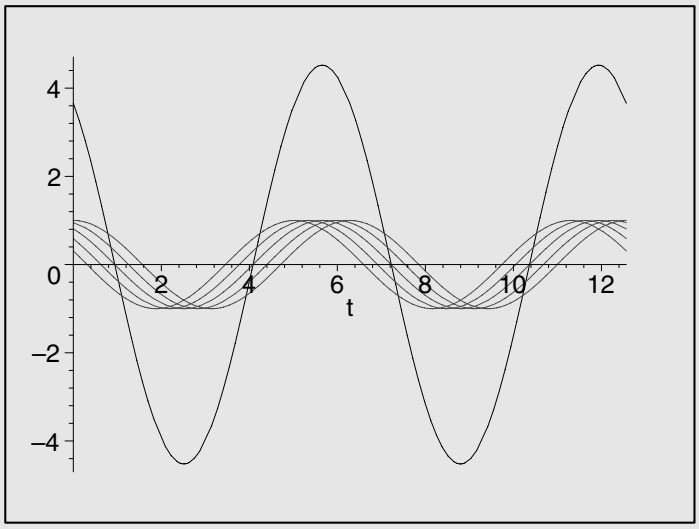
```
> psiR := add(psi[i], i=1..5);
```

$$psiR := \cos(t) + \cos(t + \phi) + \cos(t + 2\,\phi) + \cos(t + 3\,\phi) + \cos(t + 4\,\phi)$$

```
> phi := Pi/10;
```

$$\phi := \frac{\pi}{10}$$

```
> plot({seq(psi[i], i=1..5), psiR}, t=0..4*Pi);
```




```
> evalf(maximize(psiR, t=0..2*Pi));
```

$$4.520147022$$

This example illustrates that it is theoretically possible to find, graphically and numerically, the total amplitude of waves in any combination.

In the same way as the addition of two waves, we employ complex notation to derive an algebraic formula for the total amplitude of a composite of n waves. Adopting a notation similar to the above, we find that the complex amplitude of a composite wave is

$$\tilde{A}_t = A\left[1 + e^{i\varphi} + e^{i2\varphi} + \ldots + e^{i(n-1)\varphi}\right] = A\sum_{k=0}^{n-1} e^{ik\varphi}, \tag{11.13}$$

and the magnitude is again the complex scalar product of $\tilde{A}_t$,

$$A_t^2 = \tilde{A}_t\tilde{A}_t^* = A^2\frac{\cos(n\varphi) - 1}{\cos\varphi - 1}. \tag{11.14}$$

Worksheet 11.4

```
> At := sum(exp(I*k*phi), k=0..n-1);
```

$$At := \frac{e^{(n\,\phi\,I)}}{e^{(\phi\,I)} - 1} - \frac{1}{e^{(\phi\,I)} - 1}$$

```
> Epr1 := At*conjugate(At);
```

$$Epr1 := \left(\frac{e^{(n\,\phi\,I)}}{e^{(\phi\,I)}-1}-\frac{1}{e^{(\phi\,I)}-1}\right)\overline{\left(\frac{e^{(n\,\phi\,I)}}{e^{(\phi\,I)}-1}-\frac{1}{e^{(\phi\,I)}-1}\right)}$$

```
> Epr2 := evalc(Epr1):
> Epr3 := simplify(Epr2);
```

$$Epr3 := \frac{\cos(n\,\phi)-1}{\cos(\phi)-1}$$

To express this result in the way more commonly presented in other textbooks, we use the half-angle formula to rewrite equation (11.14) as

$$A_t^2 = A^2\frac{\cos(n\varphi)-1}{\cos\varphi-1} = A^2\frac{\sin^2\frac{n\varphi}{2}}{\sin^2\frac{\varphi}{2}}. \tag{11.15}$$

This mathematical formula is useful in the discussion throughout this chapter.

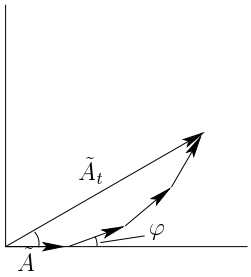


Figure 11.1: Phasor diagram.

Adding complex numbers can be represented geometrically in a phasor diagram; see Figure 11.1. In this diagram, each arrow denotes a complex number: the length of the arrow indicates the magnitude of the amplitude, and the direction of the arrow indicates the phase angle. The resultant number corresponds to a connection between the tail of the first arrow and the head of the last arrow. Both the amplitude and the phase angle of the composite can be measured geometrically in the phasor diagram.

11.3 Interference

In this section we discuss monochromatic plane waves in an idealized situation; we ignore the physical size of a slit, which we will address in relation to diffraction in the next section. Each wave is treated as a discrete source; such a wave is expressed as

$$E = E_{0z}\cos(\omega t+\varphi).$$

The y component of the electric field is treated identically, and we do not discuss it further. Two sources are described as coherent if they maintain a constant phase with respect to each other.

11.3.1 Double-slit Interference

We first discuss the double-slit experiment. The physical arrangement involves monochromatic light from a source passing a pair of slits; see Figure 11.2. Each slit can be considered a new source of waves, named S_1 and S_2. Because we ignore the physical size of the slit, a source is taken to be completely in phase at the slits.

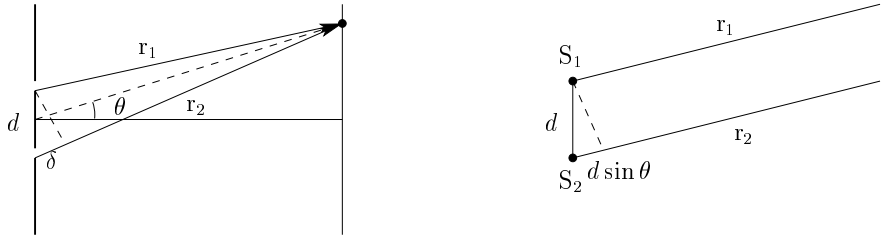


Figure 11.2: Double-slit experiment.

If we observe an interference pattern at a distance L that is much greater than the distance d between the slits, we can accept an approximation that the two rays r_1 and r_2 are parallel. The path difference δ between these two rays is (see Figure 11.2)

$$\delta = d \sin\theta. \tag{11.16}$$

One wavelength λ of path difference corresponds to a complete cycle 2π of phase difference; a path difference δ thus corresponds to a phase difference

$$\varphi = \frac{2\pi}{\lambda} d \sin\theta. \tag{11.17}$$

Throughout this chapter, one should always make the distinction between the phase angle φ and the physical angle θ.

We describe two sources S_1 and S_2 with electric fields E_1 and E_2 respectively:

$$E_1 = E_0 \cos\omega t, \quad E_2 = E_0 \cos(\omega t + \varphi).$$

According to the principle of superposition, the resultant electric field at point P is

$$E_t = E_1 + E_2 = E_0[\cos\omega t + \cos(\omega t + \varphi)]. \tag{11.18}$$

An optical instrument measures the intensity of light, which is proportional to the square of the electric field:

$$I \propto E_t^2. \tag{11.19}$$

Directly applying the mathematical formula in the preceding section to this situation, we obtain the pattern of interference for the double-slit experiment,

$$I = I_0 \cos^2 \frac{\varphi}{2}. \tag{11.20}$$

Because our objective here is to find the pattern of interference, we express our result on a relative scale; we assign a constant intensity I_0 which we discuss no further. With this formula we can find the positions of bright and dark fringes, which we will plot in a worksheet in the next section.

11.3.2 Multiple-slit Interference

If we let light pass n equally spaced slits a distance d apart, we have n sources of waves. To find the intensity at an angle θ relative to the direction of the incident wave, we must add n waves each having the same amplitude but a different phase; see Figure 11.3. Here again we ignore diffraction due to the size of the slit, and treat each wave as a discrete source.

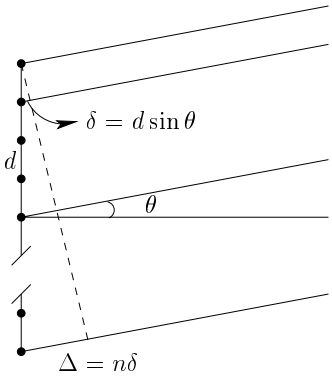


Figure 11.3: Multiple-slit experiment.

Just as for the double-slit experiment, the phase angle φ is related to the physical angle θ and the distance between two adjacent slits d,

$$\varphi = \frac{2\pi}{d} \sin\theta. \tag{11.21}$$

For n sources, we must find the resultant electric field,

$$E_t = E_0[\cos(\omega t) + \cos(\omega t + \varphi) + \cos(\omega t + 2\varphi) + \ldots + \cos(\omega t + (n-1)\varphi)]. \tag{11.22}$$

The mathematics is readily available: equation (11.15). The intensity is proportional to the square of the electric field; we directly write

$$I = I_0 \frac{\sin^2 \frac{n\varphi}{2}}{\sin^2 \frac{\varphi}{2}}. \tag{11.23}$$

We make plots of intensity for various n.

Worksheet 11.5 Instead of entering equation (11.23), to produce these plots we use the original formula

$$\frac{\cos(n\varphi) - 1}{\cos\varphi - 1},$$

which is directly derived from the summation of complex numbers using Maple as shown earlier.

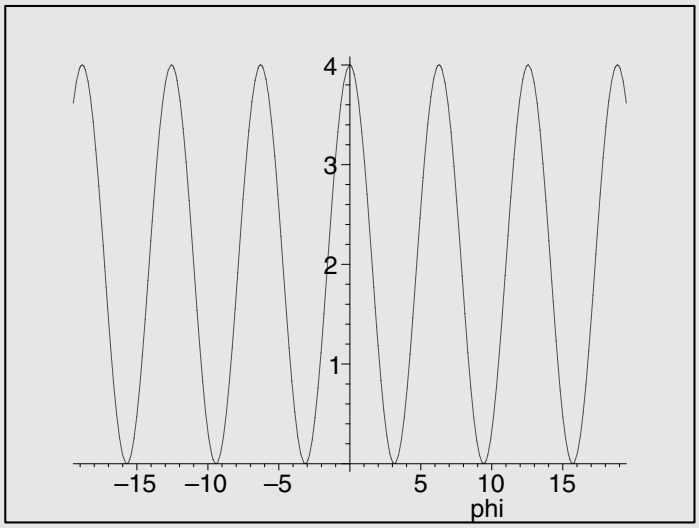
```
> At := sum(exp(I*k*phi), k=0..n-1):
> Epr1 := At*conjugate(At):
> Epr2 := evalc(Epr1):
> Epr3 := simplify(Epr2);
```

$$Epr3 := \frac{\cos(n\,\phi) - 1}{\cos(\phi) - 1}$$

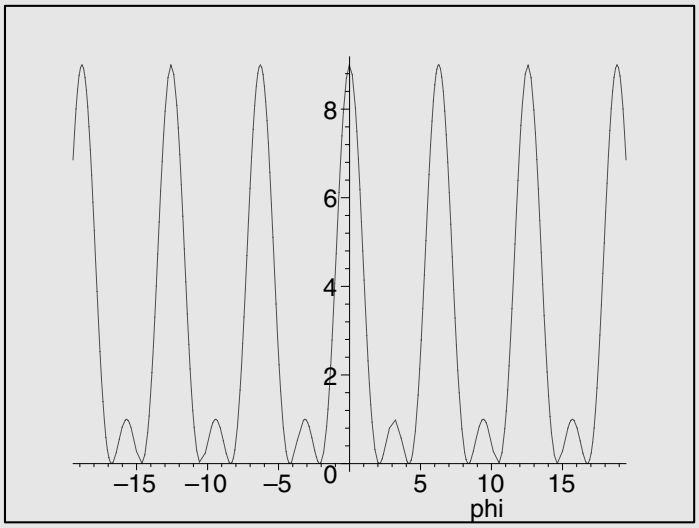
```
> Itn := unapply(Epr3, n);
```

$$Itn := n \rightarrow \frac{\cos(n\,\phi) - 1}{\cos(\phi) - 1}$$

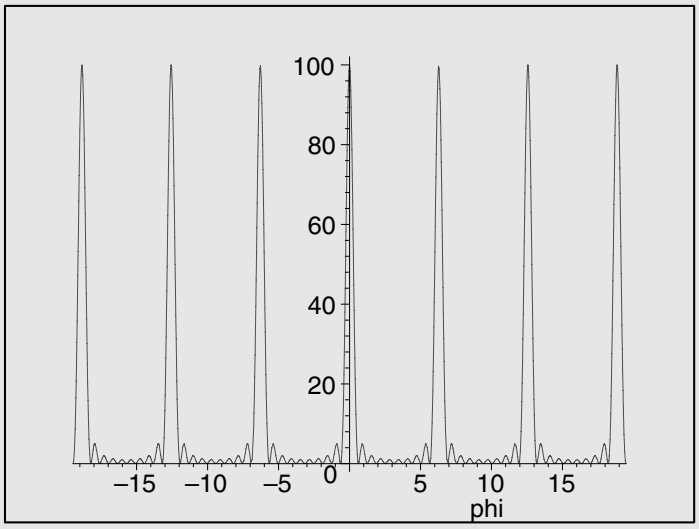
```
> plot(Itn(2), phi=-6.2*Pi..6.2*Pi);
```



```
> plot(Itn(3), phi=-6.2*Pi..6.2*Pi);
```




```
> plot(Itn(10), phi=-6.2*Pi..6.2*Pi, numpoints=200);
```



These graphs demonstrate key features of the pattern of multiple-slit interference. The positions of primary maxima, which are the greatest maxima in each graph, remain fixed, but, as n increases, the pattern becomes narrower. For $n > 2$, subsidiary maxima appear but with significantly smaller intensity.

The central maximum corresponds to $\varphi = 0$. Although at this value the denominator in equation (11.23) is zero, the intensity is finite because zero also appears in the numerator. We leave it as an exercise to prove that

$$\lim_{\varphi \to 0} \left(I_0 \frac{\sin^2 \frac{n\varphi}{2}}{\sin^2 \frac{\varphi}{2}} \right) = n^2 I_0. \tag{11.24}$$

We explain this result in a phasor diagram; see Figure 11.4. When $\varphi = 0$, all arrows align parallel in a straight line; the amplitude adds n times so that the intensity becomes n^2 times as great.

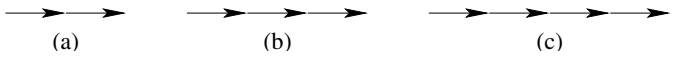


Figure 11.4: Multiple-slit phasors for constructive interference.

Because this formula is invariant with the addition of integer multiples of 2π to φ, primary maxima clearly locate at integer multiples of 2π, as is evident in the graph. The condition for a primary pattern is thus

$$\varphi = 2\pi m, \tag{11.25}$$

where m is an integer. The plot shows that the physical angle does not depend on n,

$$\sin\theta = \frac{m\lambda}{d}. \tag{11.26}$$

The condition for the first dark fringe associated with the central maximum is

$$\sin^2 \frac{n\varphi}{2} = 0, \quad \frac{n\varphi}{2} = \pi.$$

This property is also readily understandable from a phasor diagram. For n sources, there are n arrows in the phasor diagram. The first minimum corresponds to a situation in which the head of the last arrow comes back to the tail of the first arrow. We depict this condition in Figure 11.5 for interference due to (a) two slits, (b) three slits and (c) four slits.

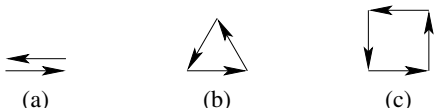


Figure 11.5: Multiple-slit phasors for destructive interference.

The geometry makes evident that

$$\varphi = \frac{2\pi}{n}. \tag{11.27}$$

In terms of the physical angle,

$$\sin\theta = \frac{\lambda}{nd}. \tag{11.28}$$

Therefore, the greater n, the narrower the pattern.

The condition for subsidiary maxima can be similarly derived, which we leave to an exercise.

11.4 Diffraction

In the preceding section we assume the width of a slit to be zero, so that a wave emerging from each slit is considered completely coherent. As such a situation is unrealistic, in this section we take into account the physical dimension of the slit. Suppose that we have a single slit of finite width a; monochromatic light passing this single slit also produces an interference pattern, generally called diffraction for this situation, although there exists no universal definition of this term.

To explain diffraction, we again use equation (11.23) for multiple slits. Referring to Figure 11.3, we consider a special case that $d \to 0$ and $n \to \infty$, but their product nd is finite, which is the width a. These sources are close together; therefore the path difference is small and the phase angle is almost zero. We define a total phase angle Φ,

$$\Phi = n\varphi, \tag{11.29}$$

which is finite. As the width a is equal to nd, the phase angle is related to the physical angle by

$$\Phi = \frac{2\pi}{\lambda} a \sin\theta. \tag{11.30}$$

Because φ is small, we use an approximation for a small angle that $\sin\varphi \cong \varphi$. With these symbols inserted into the formula for multiple slits, the intensity for a single slit becomes

$$I = 4I_{\text{max}} \left(\frac{\sin\frac{\Phi}{2}}{\Phi} \right)^2, \tag{11.31}$$

where I_{max} is $n^2 I_0$. Even though $n \to \infty$, each I_0, which is proportional to d^2, is small; thus I_{max} remains finite.

Worksheet 11.6 To employ the small-angle approximation, we invoke the `taylor` command to expand the trigonometric functions. The `denom` and `numer` commands serve to extract the denominator and numerator, respectively, of the expression.

```
> Itn := Itn0*sin(n*phi/2)^2/sin(phi/2)^2;
```

$$Itn := \frac{Itn0 \sin\left(\frac{n\,\phi}{2}\right)^2}{\sin\left(\frac{\phi}{2}\right)^2}$$

```
> phi := Phi/n;
```

$$\phi := \frac{\Phi}{n}$$

```
> Itn;
```

$$\frac{Itn0 \sin\left(\frac{\Phi}{2}\right)^2}{\sin\left(\frac{\Phi}{2\,n}\right)^2}$$

```
> Epr1 := denom(Itn);
```

$$Epr1 := \sin\left(\frac{\Phi}{2\,n}\right)^2$$

```
> Epr2 := convert(taylor(Epr1, Phi=0, 3), polynom);
```

$$Epr2 := \frac{\Phi^2}{4\,n^2}$$

```
> Itn := numer(Itn)/Epr2;
```

$$Itn := \frac{4\,Itn0 \sin\left(\frac{\Phi}{2}\right)^2 n^2}{\Phi^2}$$

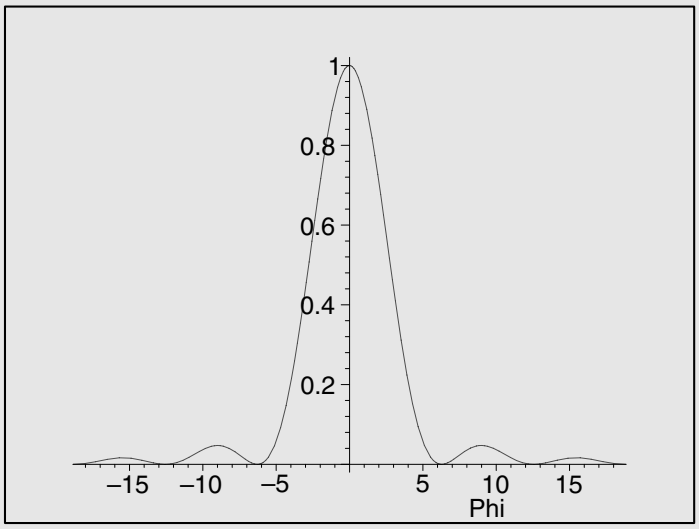
```
> Itn := algsubs(n^2*Itn0=Imax, Itn);
```

$$Itn := \frac{4 \sin\left(\frac{\Phi}{2}\right)^2 Imax}{\Phi^2}$$

```
> Imax := 1;
```

$$Imax := 1$$

```
> plot(Itn, Phi=-6*Pi..6*Pi);
```



The diffraction pattern shown above is important for our next discussion of the resolution for a single slit.

11.4.1 Resolution of Single Slits and Circular Apertures

The diffraction pattern of a single slit indicates that any source is imaged as a bright central region flanked by weaker bright and dark fringes. This wave nature of light limits an ability of optical systems, including our eyes, to discern between closely spaced objects.

Rayleigh's criterion to resolve two sources is that the first minimum of one pattern lies at the maximum of the other pattern. We calculate the first minimum from equation (11.31),

$$\sin\frac{\Phi}{2} = 0, \quad \Phi = 2\pi, \tag{11.32}$$

or as a physical angle,

$$\sin\theta = \frac{\lambda}{a}. \tag{11.33}$$

Because the angle is small, we use the small-angle approximation to obtain

$$\theta = \frac{\lambda}{a}. \tag{11.33$'$}$$

We here offer an alternative way to derive the diffraction formula, and apply this method to a circular aperture. We do not intend to be rigorous, but merely present a rudimentary introduction to advanced diffraction theory.

Understanding that diffraction involves the addition of waves of infinite number, we convert the sum to an integral. Instead of

$$E_t = A\sum_{j=0}^{n-1}\cos j\varphi, \tag{11.34}$$

we write

$$j\varphi = j\frac{2\pi d\sin\theta}{\lambda} \to z\frac{2\pi\sin\theta}{\lambda},$$

and perform the integration,

$$E_t = A\int_{-a/2}^{a/2}\cos\left(z\frac{2\pi\sin\theta}{\lambda}\right)dz = A\frac{\sin(a\pi\sin\theta/\lambda)}{\pi\sin\theta/\lambda}, \tag{11.35}$$

or, using Φ

$$I = 4I_{\max}\left[\frac{\sin\left(\frac{\Phi}{2}\right)}{\Phi}\right]^2. \tag{11.36}$$

This result is identical to equation (11.31).

Worksheet 11.7 The integration and substitution are straightforward.

```
> phi := x*2*Pi*sin(theta)/lambda;
```

$$\phi := \frac{2\,x\,\pi\sin(\theta)}{\lambda}$$

```
> Epr1 := int(Ef0*cos(phi), x=-a/2..a/2);
```

$$Epr1 := \frac{Ef0\;\lambda\sin\left(\frac{a\,\pi\sin(\theta)}{\lambda}\right)}{\pi\sin(\theta)}$$

```
> Epr2 := algsubs(2*Pi*a*sin(theta)/lambda=Phi, Epr1);
```

$$Epr2 := \frac{Ef0\;\lambda\sin\left(\frac{\Phi}{2}\right)}{\pi\sin(\theta)}$$

```
> Epr3 := subs(sin(theta)=lambda*Phi/(2*Pi*a), Epr2);
```

$$Epr3 := \frac{2\;Ef0\;a\sin\left(\frac{\Phi}{2}\right)}{\Phi}$$

```
> Epr4 := Epr3^2;
```

$$Epr4 := \frac{4\;Ef0^2\;a^2\sin\left(\frac{\Phi}{2}\right)^2}{\Phi^2}$$

```
> Itn := algsubs(Ef0^2*a^2=Imax, Epr4);
```

$$Itn := \frac{4\sin\left(\frac{\Phi}{2}\right)^2 Imax}{\Phi^2}$$

For a circular aperture, the procedure involves a similar addition of waves, but we must undertake it in two dimensions. Suppose that we have an aperture of diameter a; we describe it with polar coordinates ρ and ϕ – not to be confused with the phase angle φ. We state the fact that adding a wave in ϕ gives a Bessel function of zeroth order.[1] In contrast with a slit that involves adding cosine functions, a circular aperture thus involves adding Bessel functions.

Again we convert from a sum to an integral by

$$j\varphi \to \rho\frac{2\pi\sin\theta}{\lambda};$$

so

$$E_t = A\int_0^{a/2} J_0\left(\rho\frac{2\pi\sin\theta}{\lambda}\right)2\pi\rho d\rho = A\frac{a}{2}\frac{J_1(a\pi\sin\theta/\lambda)}{\sin\theta/\lambda}. \tag{11.37}$$

Using Maple to perform this integration, we obtain the intensity:

$$I = I_{\max}\left[\frac{J_1(\frac{\Phi}{2})}{\Phi}\right]^2. \tag{11.38}$$

This integral reflects a property of the Bessel function,

$$\int J_0(kx)x\,dx = \frac{xJ_1(kx)}{k}. \tag{11.39}$$

Worksheet 11.8 Maple can accurately evaluate this integral involving a Bessel function. The `fsolve` command is useful in finding the first minimum.

```
> phi := 2*Pi*rho*sin(theta)/lambda;
```

$$\phi := \frac{2\,\pi\,\rho\sin(\theta)}{\lambda}$$

```
> Epr1 := int(BesselJ(0,phi)*2*Pi*rho*Ef0, rho=0..a/2);
```

$$Epr1 := \frac{1}{2}\csc(\theta)\,\lambda\,Ef0\,a\,\mathrm{BesselJ}\left(1,\frac{a\,\pi\sin(\theta)}{\lambda}\right)$$

[1] Jackson 1999, p. 492.

```
> Epr2 := algsubs(2*Pi*a*sin(theta)/lambda=Phi, Epr1);
```

$$Epr2 := \frac{1}{2}\csc(\theta)\,\lambda\,Ef0\,a\,\mathrm{BesselJ}\left(1, \frac{\Phi}{2}\right)$$

```
> Epr3 := subs(csc(theta)=2*Pi*a/(lambda*Phi), Epr2);
```

$$Epr3 := \frac{\pi\,a^2\,Ef0\,\mathrm{BesselJ}\left(1, \frac{\Phi}{2}\right)}{\Phi}$$

```
> Epr4 := Epr3^2;
```

$$Epr4 := \frac{\pi^2\,a^4\,Ef0^2\,\mathrm{BesselJ}\left(1, \frac{\Phi}{2}\right)^2}{\Phi^2}$$

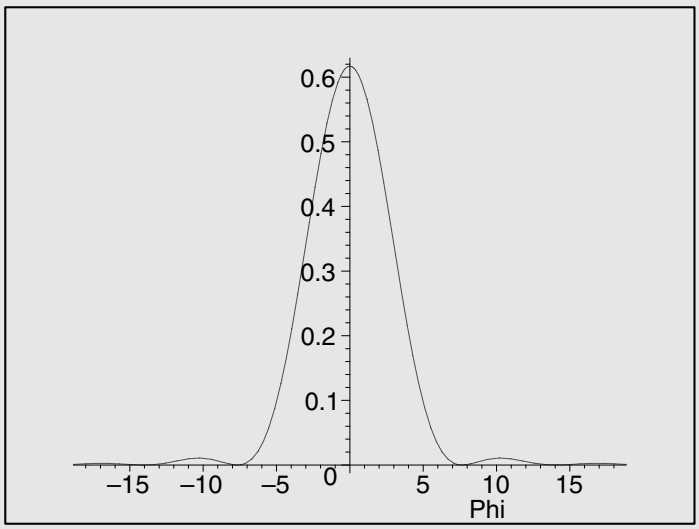
```
> Itn := algsubs(Ef0^2*a^4=Imax, Epr4);
```

$$Itn := \frac{\pi^2\,\mathrm{BesselJ}\left(1, \frac{\Phi}{2}\right)^2\,Imax}{\Phi^2}$$

```
> Imax := 1;
```

$$Imax := 1$$

```
> plot(Itn, Phi=-6*Pi..6*Pi);
```




```
> r11 := fsolve(Itn, Phi=7..8);
```

$$r11 := 7.663411940$$

```
> evalf(r11/(2*Pi));
```

$$1.219669891$$

We plot the diffraction pattern for a circular aperture, which is similar to that of a slit. The first minimum can be solved numerically, for which we obtain

$$\Phi = 7.66 = 1.22 \times \pi.$$

Therefore Rayleigh's criterion for a circular aperture of diameter a is

$$\theta = 1.22 \, \frac{\lambda}{a}. \tag{11.40}$$

This factor of 1.22 is commonly cited in introductory physics textbooks, and here we offer its derivation. We leave it as an exercise to find the next two minima, which correspond to the next two dark rings when imaging through a circular aperture.

11.5 Diffraction Grating

Among the many types of diffraction grating, one is made of an opaque glass with many equally spaced grooves cut by a diamond; the width of each slit is a and the spacing between neighboring slits is d.

We have discussed the interference pattern of ideal multiple slits, by considering the physical dimension of the slit to be zero. We have also discussed the diffraction pattern of a single slit. To apply these results to a diffraction grating, we simply combine equations (11.23) and (11.31):

$$I = 4I_{\text{max}} \frac{\sin^2 \frac{1}{2}\Phi}{\Phi^2} \frac{\sin^2 \frac{n\varphi}{2}}{\sin^2 \frac{\varphi}{2}}, \tag{11.41}$$

where we relate the phase angle to the physical angle as

$$\Phi = 2\pi \frac{a \sin\theta}{\lambda}, \quad \varphi = 2\pi \frac{d \sin\theta}{\lambda}. \tag{11.42}$$

This formula shows that the image of a diffraction grating is the pattern of an ideal multiple-slit interference enveloped by a single-slit diffraction.

From the relation between physical angle and phase angle, we see that sources with different wavelength λ appear at different locations after passing a diffraction grating. A grating therefore is useful for separating light of various wavelengths. Using Rayleigh's criterion, we derive the resolving power for this situation. Suppose that we have two sources of wavelengths λ and $\lambda' = \lambda + \Delta\lambda$; we seek a condition for λ' to have a maximum at angle θ, but λ to have a minimum at this angle. The condition for the primary features that we have derived is

$$\varphi = \frac{2\pi d \sin\theta}{\lambda'} = 2\pi m,$$

where m is called the order of the maximum, counting from 0 which corresponds to the central maximum. The condition of the first minimum for the central maximum is $\varphi = 2\pi/n$, where n is the number of slits. The first minimum associated with the mth maximum occurs then for

$$\varphi = \frac{2\pi d \sin\theta}{\lambda} = 2\pi m + \frac{2\pi}{n}.$$

Defining the resolving power R as the ratio $\lambda/\Delta\lambda$, we solve for it from the above two equations by eliminating $d\sin\theta$; we obtain

$$R \equiv \frac{\lambda}{\Delta\lambda} = mn. \tag{11.43}$$

Worksheet 11.9 In contrast to plots in previous sections, we plot the intensity versus physical angle θ. The first plot is the double-slit interference pattern with the diffraction effect. The second plot is for a ten-slit device, for two wavelengths 6.5×10^{-7} m and 5.5×10^{-7} m, corresponding to red and green light respectively.

```
> phi := 2*Pi*d*sin(theta)/lambda;
```

$$\phi := \frac{2\,\pi\,d\sin(\theta)}{\lambda}$$

```
> Phi := 2*Pi*a*sin(theta)/lambda;
```

$$\Phi := \frac{2\,\pi\,a\sin(\theta)}{\lambda}$$

```
> Itn := 4*sin(1/2*Phi)^2/Phi^2*sin(n*phi/2)^2/sin(phi/2)^2;
```

$$Itn := \frac{\sin\left(\frac{\pi\,a\sin(\theta)}{\lambda}\right)^2 \lambda^2 \sin\left(\frac{n\,\pi\,d\sin(\theta)}{\lambda}\right)^2}{\pi^2\,a^2\sin(\theta)^2\sin\left(\frac{\pi\,d\sin(\theta)}{\lambda}\right)^2}$$

```
> d := 18e-6; a := d/6;
```

$$d := 0.000018$$

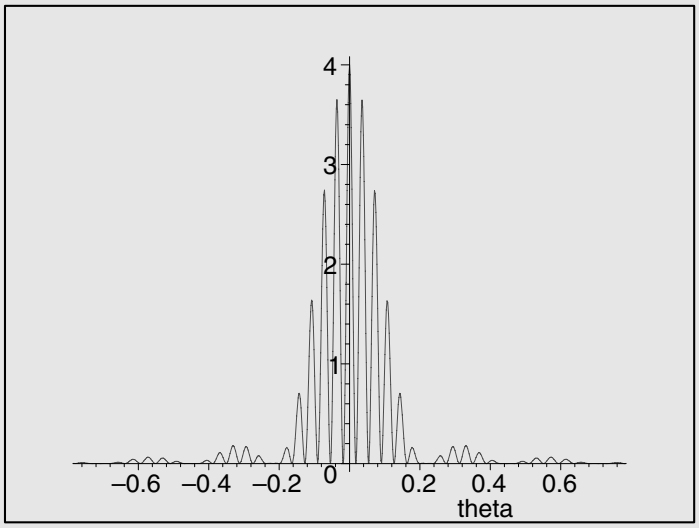
$$a := 0.3000000000\,10^{-5}$$

```
> Itn := unapply(Itn, (n, lambda));
```

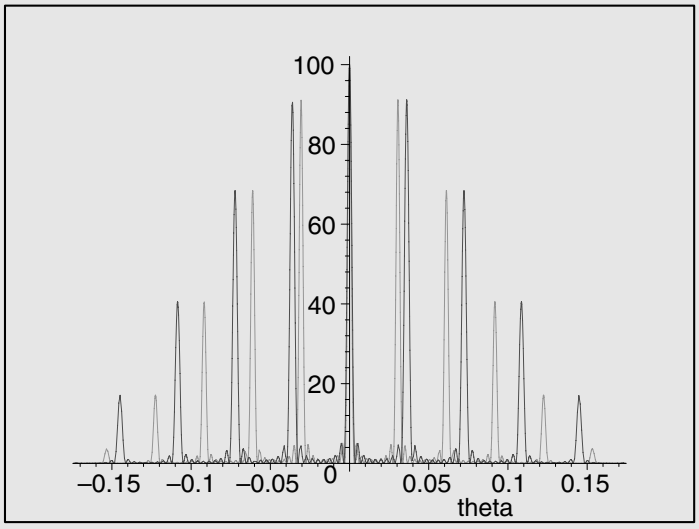
$$Itn := (n,\,\lambda)$$

$$\rightarrow \frac{0.1111111111\,10^{12}\sin\left(\frac{0.3000000000\,10^{-5}\,\pi\sin(\theta)}{\lambda}\right)^2 \lambda^2 \sin\left(\frac{0.000018\,n\,\pi\sin(\theta)}{\lambda}\right)^2}{\pi^2\sin(\theta)^2\sin\left(\frac{0.000018\,\pi\sin(\theta)}{\lambda}\right)^2}$$

```
> plot(Itn(2, 650e-9), theta=-Pi/4..Pi/4, numpoints=200);
```




```
> plot({Itn(10, 650e-9), Itn(10, 550e-9)}, theta=-Pi/18..Pi/18,
> numpoints=200);
```



From the above worksheet, as we have seen before, the greater n, the narrower the pattern, but also the intensity of subsidiary patterns decreases as m increases: this effect is due to diffraction. The plot of two superimposed wavelengths shows that they are separated; their separation increases as m increases, but there is no separation at the central pattern ($m = 0$). On this basis we can understand the formula of resolving power, $R = nm$: the greater the

product nm, the narrower the pattern and the larger the separation of patterns with distinct wavelengths, which facilitates distinguishing between two wavelengths. Because, when m increases the intensity decreases due to diffraction, in practice m cannot be too large.

11.6 Fourier Transform Spectrometry

A quantitative investigation of a spectrum involves determination of precise information about the intensity of light as a function of frequency over a broad range. A distribution of spectral intensity, $B(k)$, which is a function of intensity versus wave number or frequency, provides important information in atomic and molecular physics because each species has a unique $B(k)$. With a diffraction grating one can measure $B(k)$, but practical limits arise because, among other reasons, mechanically the number of slits n cannot be arbitrarily large.

Michelson designed an interferometer as part of an experiment to measure the speed of light at great precision in order to test the effect of the motion of the earth in the purported "ether" (the result was negative). With this instrument one can precisely measure spectra, as Michelson did in resolving the D lines of sodium atoms. According to the schematic diagram (Figure 11.6) of an interferometer, neglecting auxiliary mirrors or lenses, a beam of light is split into two rays at mirror M, which is inclined at 45° to incident light. The mirror M, called a beam splitter, transmits half the light incident on it and reflects the rest. One ray is reflected from M vertically upward towards mirror M_1 the distance of which from M is adjustable; the second ray is transmitted horizontally through M towards a fixed mirror M_2. After reflecting from M_1 and M_2, the two rays reunite at M to produce an interference pattern, which one can view through a telescope. A compensating plate P of the same thickness and material as M is placed in the horizontal ray to ensure that the two returning rays travel through the same thickness of the material of the beam splitter. In general, M_1 and M_2 are not equidistant from M.

The pattern of intensity for the double-slit experiment conforms to

$$I = I_0 \cos^2 \frac{\varphi}{2}. \tag{11.44}$$

In a Michelson interferometer, one can vary the position of M_1, which is equivalent to varying φ in the above formula, because

$$\varphi = \frac{2\pi}{\lambda} x = kx. \tag{11.45}$$

A plot of the intensity versus the difference in the optical paths from M to M_1 and to M_2 is called an interferogram. For an electromagnetic wave of a particular frequency, the interferogram is described by this function:

$$I = I_0 \cos^2 \frac{kx}{2} = \frac{I_0}{2}[1 + \cos(kx)]. \tag{11.46}$$

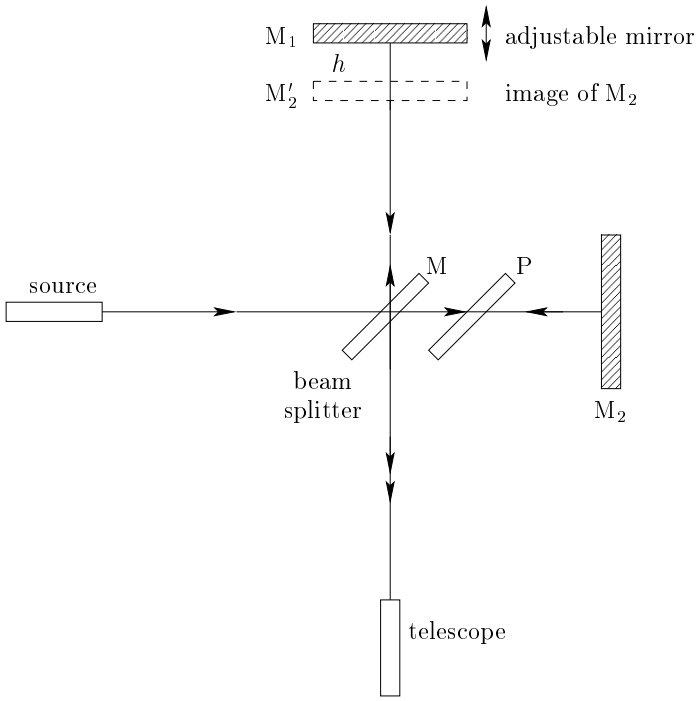


Figure 11.6: Michelson interferometer.

For an electromagnetic wave with a distribution $B(k)$ of spectral intensity, the interferogram is an integral over all frequencies, neglecting the constant term $I_0/2$ as it is simply an offset:

$$I(x) = \frac{1}{(2\pi)^{1/2}} \int_0^\infty B(k) \cos(kx) dk. \tag{11.47}$$

Conversely, if we have an interferogram, the spectrum $B(k)$ is

$$B(k) = \frac{1}{(2\pi)^{1/2}} \int_0^\infty I(x) \cos(kx) dx. \tag{11.48}$$

Therefore $I(x)$ and $B(k)$ are simply cosine Fourier transforms of each other.

Recall the uncertainty relation,

$$\Delta x \Delta k \geq \frac{1}{2}; \tag{11.49}$$

in order to decrease Δk, we must increase Δx. We can hence measure the frequency more precisely by letting the mirror move a greater distance. Although Michelson's idea is brilliant, the full potential of this method had to await the advent of an electronic digital computer to rapidly calculate a Fourier transform. A Michelson interferometer is currently the basis of many instruments used for precise measurement.

Example 11.2 With this example we illustrate the cosine Fourier transformation. Suppose a spectrum is described by this function:

$$B(k) = \exp\left[-\frac{(k-k_1)^2}{2a^2}\right] + 0.7\exp\left[-\frac{(k-k_2)^2}{2a^2}\right],$$

which represents a situation in which a spectrum has two closely spaced lines of wave numbers k_1 and k_2, for each line of which the profile is Gaussian. To evaluate the interferogram, we perform an integration

$$I(x) = \Re\left\{\frac{1}{(2\pi)^{1/2}}\int_0^\infty B(k)e^{ikx}dk\right\}.$$

Worksheet 11.10 We take arbitrary values $k_1 = 15$, $k_2 = 13$ and $a = 0.25$ to produce a plot.

```
> a := 0.25;
```

$$a := 0.25$$

```
> k1 := 15;
```

$$k1 := 15$$

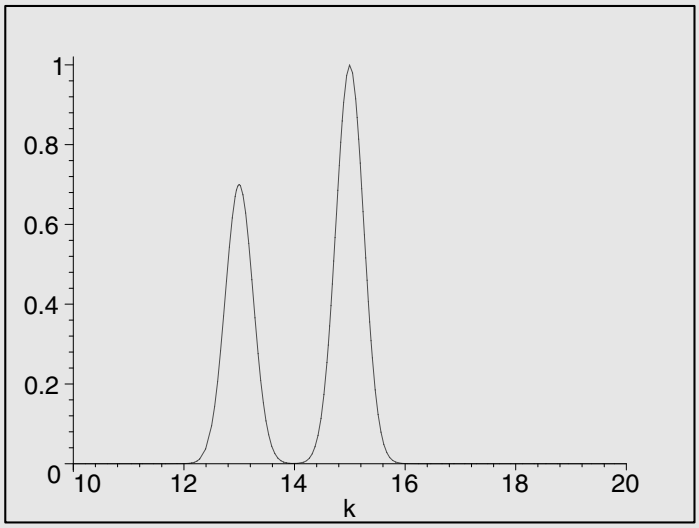
```
> k2 := 13;
```

$$k2 := 13$$

```
> B1 := 1*exp(-(k - k1)^2/(2*a^2)) + 0.7*exp(-(k - k2)^2/(2*a^2));
```

$$B1 := e^{(-8.000000000\,(k-15)^2)} + 0.7\,e^{(-8.000000000\,(k-13)^2)}$$

```
> plot(B1, k=10..20);
```

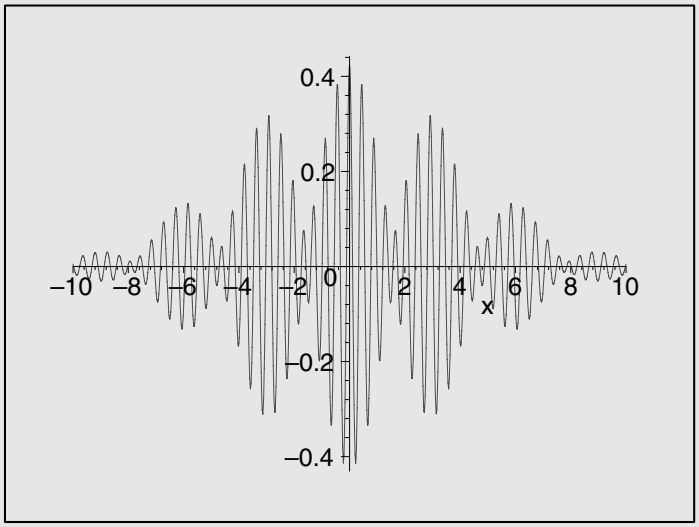


```
> Epr1 := 1/sqrt(2*Pi)*int(B1*exp(I*k*x), k=0..infinity);
```

$$Epr1 := \frac{1}{2}\sqrt{2}(0.3133285343\,\%1\,(e^{(1.\,I\,x)})^{15} + 0.2193299740\,\%1\,(e^{(1.\,I\,x)})^{13} + 0.3133285343\,\%1\,(e^{(1.\,I\,x)})^{15}\,\mathrm{erf}(0.1767766953\,I\,x + 42.42640687) + 0.2193299740\,\%1\,(e^{(1.\,I\,x)})^{13}\,\mathrm{erf}(0.1767766953\,I\,x + 36.76955262))\,/\sqrt{\pi}$$

$$\%1 := e^{(-0.03125000000\,x^2)}$$

```
> plot(Re(Epr1), x=-10..10, numpoints=400); #takes a while
```



The interferogram resembles a beat pattern that would be obtained by adding two waves of distinct frequencies, which is exactly what it is. The original spectral lines are enveloped by a Gaussian function. The Fourier transform of a Gaussian function is also a Gaussian function; the interferogram thus appears to be enveloped by a Gaussian function as well. Although Michelson lacked a digital computer to calculate such a Fourier transform, based on the above reasoning he carefully examined interferograms recorded from visual observations and deduced correctly that many spectral lines, such as a green line of atomic mercury at 546.1 nm, are multiplets comprising two or more closely spaced components, because the interferograms show a pattern of beats.

11.7 Fresnel Diffraction

In previous sections, we have restricted our discussion to the approximation that all rays passing a slit are parallel to one another. Placing a screen far from the slit fulfils this condition; this type of problems is called Fraunhofer diffraction.

We now consider a situation in which light enters from infinity, casting the shadow of an opaque object on a screen; see Figure 11.7. As the screen is not far from the object, we can no longer assume that rays are parallel after the object. Near the edge of the shadow, we see also a diffraction pattern. This type of problem is called Fresnel diffraction.

The intensity at P can be calculated by the addition of sources from D up to infinity, and down to the edge of the object. We must calculate the path difference between FP and DP. Because only sources near D make a significant contribution, an approximation that $FP-DP$ is $h^2/2s$ is satisfactory. The phase difference for Fresnel diffraction is therefore proportional to the *square* of the distance from a reference point D; for comparison with problems of Fraunhofer diffraction, the phase difference is linearly proportional to h.

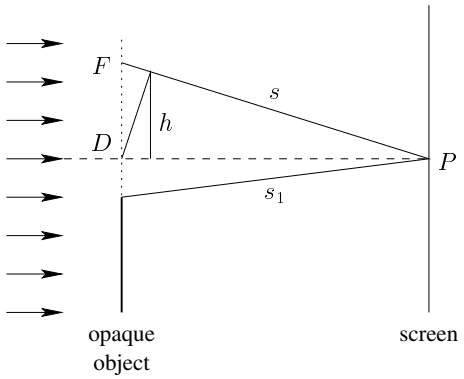


Figure 11.7: Fresnel diffraction.

Any problem of diffraction can, in principle, be solved geometrically on constructing a phasor diagram. In this case, we prepare a phasor diagram, which is a curve formed on addition of many infinitesimal vectors according to a requirement that the angle increases as the square of the length of the curve. We define a parameter η,

$$\eta^2 = \frac{2\pi}{\lambda}\frac{h^2}{2s}. \tag{11.50}$$

Hence each vector is

$$e^{i\eta^2}.$$

Adding these vectors yields a curve described by this integral,

$$E_t = \sqrt{\frac{2}{\pi}}\int_0^w e^{i\eta^2}d\eta. \tag{11.51}$$

As our concern is only the relative intensity, a factor $\sqrt{2/\pi}$ has no particular significance. With this choice, the integral converges to $\pm(1/2 + i/2)$. This curve is called the Cornu spiral.

To find the intensity, we measure the distance in the phasor diagram. The Cornu spiral in the complex plane is expressed with x and y in a parametric form with w,

$$x = \Re\left\{\sqrt{\frac{2}{\pi}}\int_0^w e^{i\eta^2}d\eta\right\},$$

$$y = \Im\left\{\sqrt{\frac{2}{\pi}}\int_0^w e^{i\eta^2}d\eta\right\}.$$

Let the distance between D and the edge of the object be z, which is linearly proportional to w; specifically,

$$w = -z\sqrt{\frac{\pi}{\lambda s}}.$$

Suppose that we seek the intensity at point P: we let D correspond to the center of the Cornu spiral $(0,0)$. We add from D up to infinity, which corresponds to $(1/2,1/2)$, and from D down only to the object, corresponding to (x,y). The intensity then corresponds to the square of the distance:

$$I \propto \left[\left(x-\frac{1}{2}\right)^2+\left(y-\frac{1}{2}\right)^2\right].$$

For $w>0$, so that $x<0$ and $y<0$, the intensity has an oscillatory pattern, depending on z, or w. For $w<0$, corresponding to the shadow region, for which $x>0$ and $y>0$, we employ only one end of the Cornu spiral; the intensity falls off monotonically. The intensity exactly opposite the edge is, from the graph, $1/4$ of that of the incident light.

Worksheet 11.11 Defining the integral functions, we plot the Cornu spiral. We evaluate the integrals numerically and plot the pattern of diffraction. We employ `Heaviside` for graphic purposes only to indicate the opaque object; this command is useful in differential equations to produce the step function.

```
> assume(u, real); assume(v, real);
> Amp := sqrt(2/Pi)*int(exp(I*u^2), u=0..v);
```

$$Amp := \left(\frac{1}{2}+\frac{1}{2}I\right)\operatorname{erf}\left(\left(\frac{1}{2}-\frac{1}{2}I\right)\sqrt{2}\,v\right)$$

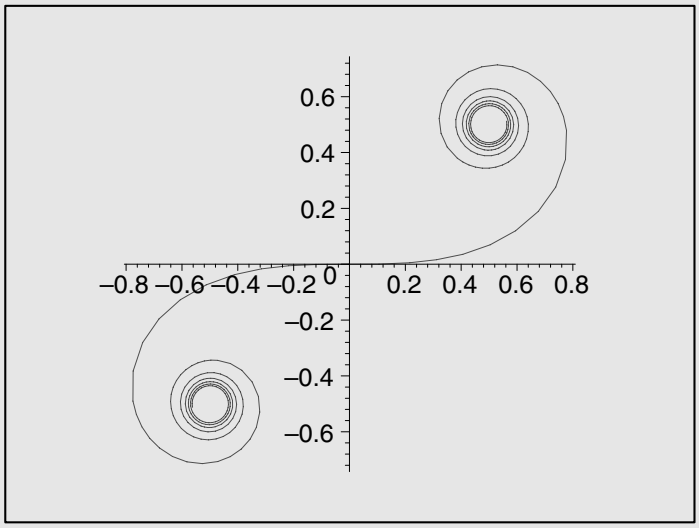
```
> x := Re(Amp);
```

$$x := \Re\left(\left(\frac{1}{2}+\frac{1}{2}I\right)\operatorname{erf}\left(\left(\frac{1}{2}-\frac{1}{2}I\right)\sqrt{2}\,v\right)\right)$$

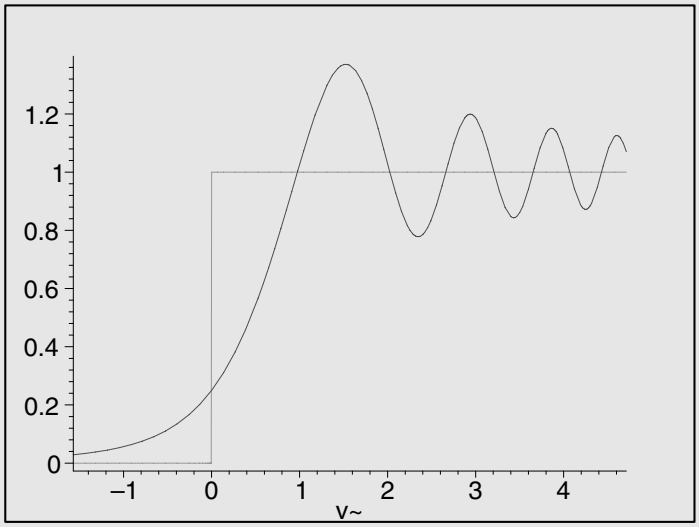
```
> y := Im(Amp);
```

$$y := \Im\left(\left(\frac{1}{2}+\frac{1}{2}I\right)\operatorname{erf}\left(\left(\frac{1}{2}-\frac{1}{2}I\right)\sqrt{2}\,v\right)\right)$$

```
> plot([x, y, v=-2*Pi..2*Pi], scaling=constrained);
```




```
> plot({1/2*((x + 0.5)^2 + (y + 0.5)^2), Heaviside(v)},
> v=-Pi/2..3/2*Pi, axes=frame);
```



Exercises

1. Modify the worksheet in Section 11.1.1, and observe polarizations for the following conditions:

   (a) linear polarization, for which $E_{0y} = 5$, $E_{0z} = 5/2$, $\alpha_z - \alpha_y = 0$;

   (b) elliptical polarization, for which $E_{0y} = 5$, $E_{0z} = 5/2$, $\alpha_z - \alpha_y = \pi/3$;

   (c) circular polarization, for which $E_{0y} = 5$, $E_{0z} = 5$, $\alpha_z - \alpha_y = \pi/2$.

2. Verify equation (11.24).

3. From the formula for ideal multiple-slit interference, find the position and intensity of subsidiary maxima.

4. To understand Rayleigh's criterion, we consider equation (11.31) for two sources:

$$I = 4\left[\frac{\sin\left(\frac{\Phi-\frac{\delta}{2}}{2}\right)}{\Phi-\frac{\delta}{2}}\right]^2 + 4\left[\frac{\sin\left(\frac{\Phi+\frac{\delta}{2}}{2}\right)}{\Phi+\frac{\delta}{2}}\right]^2. \tag{11.52}$$

   When the first minimum from one source resides at the maximum of the other source, it corresponds to $\delta = 2\pi$; make a plot of this condition, which should resemble Figure 11.8. Make plots for $\delta > 2\pi$ and $\delta < 2\pi$. Rayleigh's criterion for a circular aperture can be similarly obtained using equation (11.38).

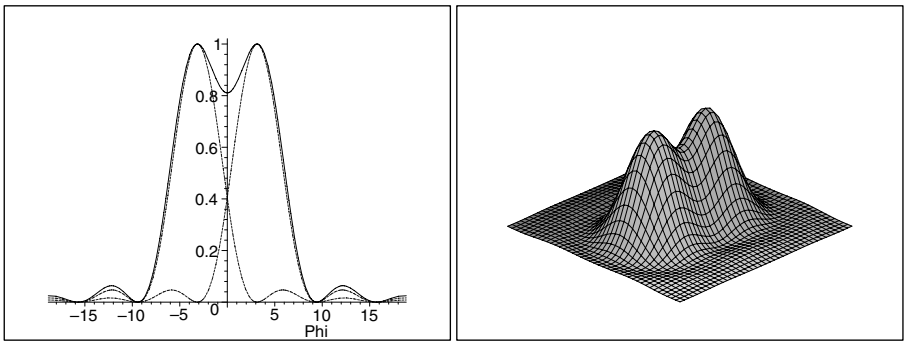


Figure 11.8: Rayleigh's criterion for a single slit and a circular aperture.

5. In Section 11.4.1, the angular size of the first dark ring of the diffraction pattern formed by a circular aperture is found to be

$$\sin\theta_1 = 1.22\frac{\lambda}{a}.$$

Prove that the the angular sizes of the second and third dark rings are

$$\sin\theta_2 = 2.23\frac{\lambda}{a}, \quad \sin\theta_3 = 3.24\frac{\lambda}{a}.$$

Hint: find the roots of the Bessel function of order 1.

6. Sketch the combined pattern for diffraction and interference of light of wavelength 650.0 nm passing four slits of width 3.0 μm and separated by 9.0 μm.

7. When the size of an aperture is much greater than the wavelength of the light, it is useful to introduce the concept of *rays*, along which the light travels. Geometrical optics is concerned with the determination of these rays, and according to Fermat's principle, light travels between two points along a path that requires the least time compared to other nearby paths. We assume that the speed of light in glass is lower than the speed of light in air by a factor n, the index of refraction. Referring to Figure 11.9, we attempt to find the position of C such that PCQ corresponds to the least time, compared with a path PRQ or PSQ, for instance.

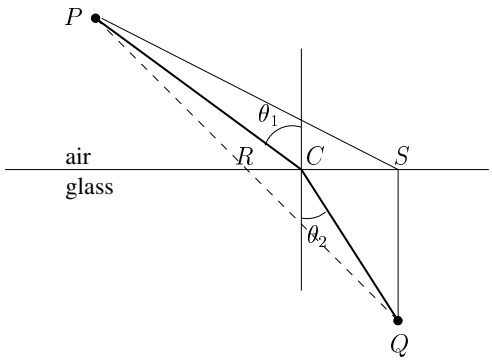


Figure 11.9: Snell's law using Fermat's principle.

(a) We first use a numerical example: let the coordinates of P, Q, C be $(-5, 5)$, $(5, -5)$, $(x, 0)$, respectively, all have units of meters. We also assume that the speed of light in air is 3×10^8 m s^{-1}, and the index of glass n is 1.5. The time required for the light to travel from P to Q is thus

$$t = \frac{\sqrt{[x-(-5)]^2 + 5^2}}{c} + \frac{\sqrt{(5-x)^2 + 5^2}}{c/n}.$$

Plot t as a function of x, and find the value of x that minimizes t.
Answer: $x_{\text{min}} = 1.81$ m.

(b) Let the coordinates of P, Q, C be (a, b), (d, e), $(x, 0)$, respectively, the time it takes to travel from P to Q is

$$t = \frac{\sqrt{(a-x)^2 + b^2}}{c} + \frac{\sqrt{(d-x)^2 + e^2}}{c/n}. \tag{11.53}$$

Take the derivative of t with respect to x and set the derivation equal to zero, verify that

$$\frac{(x-a)}{\sqrt{(x-a)^2 + b^2}} = \frac{n(d-x)}{\sqrt{(d-x)^2 + e^2}}, \tag{11.54}$$

which is equivalent to

$$\sin\theta_1 = n \sin\theta_2; \tag{11.55}$$

This is known as Snell's law of refraction.

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12 Special Relativity

The treatment of relativity in the physics literature is abundant. The most common obstacle to understanding relativity is confusion about observers in different frames. In this chapter, we attempt to present relativity in a uniform fashion. We use matrix algebra to perform a change of inertial frames. Our major concern is to be logically consistent; to do so we avoid arguments such as switching places, and we solve equations directly. Although our approach might result in lengthier calculations, we take advantage of the solving power of Maple to facilitate this task.

12.1 Lorentz Transformation

The origin of special relativity lies in electromagnetism. Maxwell's equations are not invariant under the Galilean transformation, a prerequisite of Newtonian mechanics. Lorentz derived a set of transformations under which Maxwell's equations are invariant.

Let us consider two inertial reference systems K and K' with coordinate axes xyz and $x'y'z'$, in which the system K' moves relative to K along the $x(x')$ axis with velocity u. The Lorentz transformations are

$$x' = \frac{x - ut}{\sqrt{1 - u^2/c^2}}, \quad y' = y, \quad z' = z, \quad t' = \frac{t - ux/c^2}{\sqrt{1 - u^2/c^2}}. \tag{12.1}$$

The Galilean transformation is the limit of $c \to \infty$. We can express these transformations in a matrix form. Defining

$$\beta \equiv \frac{u}{c}, \quad \gamma \equiv \frac{1}{\sqrt{1 - u^2/c^2}} \tag{12.2}$$

and

$$x^0 \equiv ct, \quad x^1 = x, \quad x^2 = y, \quad x^3 = z, \tag{12.3}$$

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(the superscripts are indices, not exponents), this notation allows us to write equation (12.1) as

$$\begin{pmatrix} x'^0 \\ x'^1 \\ x'^2 \\ x'^3 \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma\beta & 0 & 0 \\ -\gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \end{pmatrix}, \tag{12.4}$$

or more abstractly

$$\mathbf{x}' = \mathbf{L}\mathbf{x}, \tag{12.5}$$

where $\mathbf{x}$ and $\mathbf{x}'$ are column matrices containing four components of the corresponding vectors, and $\mathbf{L}$ is a square matrix.

From the contribution of Minkowski and Einstein, we recognize that space and time are inseparable. Three spatial dimensions and one temporal dimension form a four-dimensional space–time, or the Minkowski space. A point (ct, x, y, z) in the Minkowski space is called an *event*, and the trajectory of a particle in the Minkowski space is called a *world line*.

We define a four-vector as a set of four quantities that conform to the Lorentz transformations,

$$\begin{pmatrix} a'^0 \\ a'^1 \\ a'^2 \\ a'^3 \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma\beta & 0 & 0 \\ -\gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a^0 \\ a^1 \\ a^2 \\ a^3 \end{pmatrix}. \tag{12.6}$$

In the same way we use an abstract notation to express the above equation:

$$\mathbf{a}' = \mathbf{L}\mathbf{a}. \tag{12.7}$$

In Section 6.2, we urge the reader to be aware of the basis for a vector in matrix form. In the Minkowski space, the basis vectors for a four-vector consist of three Cartesian basis vectors and one basis vector parallel to the coordinate of time t. In this chapter we work exclusively on components, arranging them in a matrix, without referring to basis vectors. We may alternatively think of this matrix representation as writing a system of four equations in a compact notation.

A four-vector scalar product is defined as

$$-a^0b^0 + a^1b^1 + a^2b^2 + a^3b^3; \tag{12.8}$$

be aware of the minus sign for the zeroth (temporal) component. This quantity is invariant under the Lorentz transformation; we verify this fact by a direct calculation.

Worksheet 12.1 In this worksheet we invoke the `LinearAlgebra` package. The matrix of the Lorentz transformation is defined as `L`. Be aware that `gamma` is defined as Euler's constant in Maple; we avoid using this name by assigning γ to `gma`. Four-vectors $\mathbf{a}$ and $\mathbf{b}$ are denoted `A` and `B`, respectively. In the K' frame, we use `Ap` and `Bp` to represent them.

```
> with(LinearAlgebra):
> gma := 1/sqrt(1 - beta^2):
> L := << gma | -gma*beta | 0 | 0 >, < -gma*beta | gma | 0 | 0 >,
< 0 | 0 | 1 | 0 >, < 0 | 0 | 0 | 1 >>;
```

$$L := \begin{bmatrix} \frac{1}{\sqrt{1-\beta^2}} & -\frac{\beta}{\sqrt{1-\beta^2}} & 0 & 0 \\ -\frac{\beta}{\sqrt{1-\beta^2}} & \frac{1}{\sqrt{1-\beta^2}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

```
> A := < a0, a1, a2, a3 >;
```

$$A := \begin{bmatrix} a0 \\ a1 \\ a2 \\ a3 \end{bmatrix}$$

```
> B := < b0, b1, b2, b3 >;
```

$$B := \begin{bmatrix} b0 \\ b1 \\ b2 \\ b3 \end{bmatrix}$$

```
> Ap := L.A;
```

$$Ap := \begin{bmatrix} \frac{a0}{\sqrt{1-\beta^2}} - \frac{\beta\, a1}{\sqrt{1-\beta^2}} \\ -\frac{\beta\, a0}{\sqrt{1-\beta^2}} + \frac{a1}{\sqrt{1-\beta^2}} \\ a2 \\ a3 \end{bmatrix}$$

```
> Bp := L.B;
```

$$Bp := \begin{bmatrix} \frac{b0}{\sqrt{1-\beta^2}} - \frac{\beta\, b1}{\sqrt{1-\beta^2}} \\ -\frac{\beta\, b0}{\sqrt{1-\beta^2}} + \frac{b1}{\sqrt{1-\beta^2}} \\ b2 \\ b3 \end{bmatrix}$$

```
> simplify(-Ap[1]*Bp[1] + Ap[2]*Bp[2] + Ap[3]*Bp[3] + Ap[4]*Bp[4]);
```

$$a1\ b1 - a0\ b0 + a2\ b2 + a3\ b3$$

We find that

$$-a'^0 b'^0 + a'^1 b'^1 + a'^2 b'^2 + a'^3 b'^3 = -a^0 b^0 + a^1 b^1 + a^2 b^2 + a^3 b^3. \tag{12.9}$$

We can simply bear in mind that there is a minus sign for the temporal component when performing a four-vector scalar product. However, to be more systematic in tracking the minus sign, and to prepare for more sophisticated constructions for general relativity in Chapter 18, we introduce a *covariant* four-vector a_μ, which differs from a *contravariant* four-vector a^μ by a minus sign in the temporal component:

$$a^\mu = \begin{pmatrix} a^0 \\ a^1 \\ a^2 \\ a^3 \end{pmatrix}, \quad a_\mu = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} \equiv \begin{pmatrix} -a^0 \\ a^1 \\ a^2 \\ a^3 \end{pmatrix}. \tag{12.10}$$

The description of vectors of these two types might be misleading; we employ the terminology merely to distinguish the position of indices, namely "contravariant" for superscripts, and "covariant" for subscripts. The physical distinction between contravariant and covariant vectors lies in the transformation rules to which they are subject, a topic beyond the scope of this book. We define the metric tensor,

$$g_{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{12.11}$$

so that we can lower the index of a contravariant vector to form a covariant vector,

$$a_\mu = \sum_{\nu=0}^{3} g_{\mu\nu} a^\nu, \tag{12.12}$$

or explicitly

$$a_\mu = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} \equiv \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a^0 \\ a^1 \\ a^2 \\ a^3 \end{pmatrix} = \begin{pmatrix} -a^0 \\ a^1 \\ a^2 \\ a^3 \end{pmatrix}. \tag{12.13}$$

The scalar product using the above notation becomes

$$\sum_{\mu=0}^{3} a_\mu b^\mu.$$

Adopting the Einstein summation convention, we further suppress the summation symbol:

$$a_\mu b^\mu.$$

Repetition of a Greek index in a product implies summation; for example, equation (12.12) becomes $a_\mu = g_{\mu\nu} a^\nu$. This notation is particularly convenient in general relativity; according to an anecdote, Einstein regarded it as his "great discovery in mathematics."

The reader should not be concerned if the above definitions seem unfamiliar; we have no particular need of this knowledge for the rest of this chapter. In summary, a four-vector can be represented by its four components arranged in a column matrix, and they are subject to the Lorentz transformation. Some examples of four-vectors are

- space–time interval: $x^\mu_{\mathcal{B}} - x^\mu_{\mathcal{A}}$;
- wave frequency and wave vector: $(\omega/c,\ k^1,\ k^2,\ k^3)$;
- relativistic energy and momentum: $p^\mu = (E/c,\ p^1,\ p^2,\ p^3)$.

We apply transformation properties of four-vectors in subsequent sections. The most important aspect of special relativity is to distinguish between the primed system, K', and the unprimed system, K. Much confusion about relativity arises from the question of who is moving. Throughout this chapter we use a consistent notation. That is, *we* are situated in the K frame, and *we* consider *ourselves* at rest; *we* see that K' is moving in the x direction, coinciding with x', at velocity u. Although observers situated in the K' frame consider *themselves* at rest, and *they* consider us moving, we emphasize that *their* perception of who is moving is irrelevant to *our* discussion in this section. Hence *we* seek to know how a physical quantity measured by *us* in the rest frame K, denoted without a prime, is related to that measured by *them* in a moving frame K', denoted with a prime. Thus the mathematical objective is always to express unprimed parameters in terms of primed ones and u. One must clearly understand this objective before proceeding to a calculation.

12.1.1 Length Contraction and Time Dilation

The simplest four-vector is the interval between two Minkowski events,

$$(c\Delta t, \Delta x, \Delta y, \Delta z) = (ct_B, x_B, y_B, z_B) - (ct_A, x_A, y_A, z_A),$$

which is subject to the Lorentz transformation.

Considering the effect of length contraction of a moving object: we seek to know the length of a moving rod as it appears to a stationary observer. We analyze the problem in the following way. Suppose the rod to be at rest in the K' frame; *we* see the K' frame move parallel to the x axis at velocity u. *We* measure the length by identifying two simultaneous events in K: one end of the rod passes at $(ct_1, x_1, 0, 0)$, and the other end of the rod passes at $(ct_1, x_2, 0, 0)$. The length according to *us* is $\Delta x = x_2 - x_1$. These two events are viewed in the K' frame as $(ct'_1, x'_1, 0, 0)$ and $(ct'_2, x'_2, 0, 0)$. Because the rod is at rest in the K' frame, x'_1 and x'_2 are two fixed values. The length measured by an observer in the K' frame is therefore $\Delta x' = x'_2 - x'_1$, although t'_2 might differ from t'_1. The objective of this problem is to elucidate the relation between Δx (unprimed) and $\Delta x'$ (primed), in terms of the latter, when $\Delta t = 0$, or simultaneously in K.

The transformation of a space–time interval is

$$\Delta \mathbf{x}' = \mathbf{L}\, \Delta \mathbf{x}. \tag{12.14}$$

The result is

$$\Delta t' = \frac{\Delta t - \beta \Delta x/c}{\sqrt{1-\beta^2}}, \tag{12.15a}$$

$$\Delta x' = \frac{\Delta x - \beta c \Delta t}{\sqrt{1-\beta^2}}, \tag{12.15b}$$

$$\Delta y' = \Delta y, \tag{12.15c}$$

$$\Delta z' = \Delta z. \tag{12.15d}$$

The solution of Δx when $\Delta t = 0$, in terms of $\Delta x'$, is readily obtained from equation (12.15b). For this problem, one requires no knowledge of $\Delta t'$. We have

$$\Delta x = \Delta x' \sqrt{1 - u^2/c^2}. \tag{12.16}$$

Recall that $\Delta x'$ is the length of the rod according to an observer in K', who has no motion relative to it. We conclude that a moving object becomes shortened.

Worksheet 12.2 In this worksheet we use `txyz`, with components `(c*dt, dx, dy, dz)` to denote the four-vector of the space–time interval, $(c\Delta t, \Delta x, \Delta y, \Delta z)$. We perform the Lorentz transformation to obtain the components of the space–time interval in the primed system, represented by `txyzp`. We then evaluate at `dt=0` in `Eq3` to obtain `dx` in `Eq4`.

```
> with(LinearAlgebra):
> gma := 1/sqrt(1 - beta^2):
> L := << gma | -gma*beta | 0 | 0 >, < -gma*beta | gma | 0 | 0 >,
< 0 | 0 | 1 | 0 >, < 0 | 0 | 0 | 1 >>;
```

$$L := \begin{bmatrix} \frac{1}{\sqrt{1-\beta^2}} & -\frac{\beta}{\sqrt{1-\beta^2}} & 0 & 0 \\ -\frac{\beta}{\sqrt{1-\beta^2}} & \frac{1}{\sqrt{1-\beta^2}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

```
> txyz := < c*dt, dx, dy, dz >;
```

$$txyz := \begin{bmatrix} c\,dt \\ dx \\ dy \\ dz \end{bmatrix}$$

```
> txyzp := L.txyz:
```

```
> txyzp := map(simplify, txyzp);
```

$$txyzp := \begin{bmatrix} \dfrac{c\,dt - \beta\,dx}{\sqrt{1-\beta^2}} \\ -\dfrac{\beta\,c\,dt - dx}{\sqrt{1-\beta^2}} \\ dy \\ dz \end{bmatrix}$$

```
> Eq1 := dtp = txyzp[1]/c;
```

$$Eq1 := dtp = \frac{c\,dt - \beta\,dx}{\sqrt{1-\beta^2}\,c}$$

```
> Eq2 := dxp = txyzp[2];
```

$$Eq2 := dxp = -\frac{\beta\,c\,dt - dx}{\sqrt{1-\beta^2}}$$

```
> Eq3 := eval(Eq2, dt=0);
```

$$Eq3 := dxp = \frac{dx}{\sqrt{1-\beta^2}}$$

```
> Eq4 := isolate(Eq3, dx);
```

$$Eq4 := dx = dxp\,\sqrt{1-\beta^2}$$

We next consider the effect of time dilation for a moving frame. Suppose a clock to be at rest in the K' frame. The interval between two events $\mathcal{A}'$ $(ct'_3, x'_3, 0, 0)$ and $\mathcal{B}'$ $(ct'_4, x'_3, 0, 0)$ in the K' frame is $\Delta t' = t'_4 - t'_3$. We seek to evaluate this interval according to a stationary observer in K who sees K' move at velocity u. To do so we must find the unprimed events $\mathcal{A}$ $(ct_3, x_3, 0, 0)$ and $\mathcal{B}$ $(ct_4, x_4, 0, 0)$ in the K frame, and $\Delta t = t_4 - t_3$ is our desired quantity (unprimed).

The transformation of a space–time interval is the same as above. Our objective is again to evaluate unprimed parameters in terms of primed ones. There is a subtle difference between this problem and that above: to find Δt, we must also find $\Delta x = x_4 - x_3$, which is not zero; the reason is that the clock in K' is moving according to *us*. We need first to solve Δx of equation (12.15b) under the condition $\Delta x' = 0$:

$$\Delta x = \beta c \Delta t.$$

This result is understandable because the distance that the clock moves (Δx) is equal to the velocity of the frame ($\beta c = u$) times the time interval (Δt), all according to *us*. Substituting Δx into equation (12.15a), we obtain

$$\Delta t = \frac{\Delta t'}{\sqrt{1 - v^2/c^2}}. \tag{12.17}$$

Therefore Δt is always greater than $\Delta t'$, and we conclude that a moving clock runs slowly.

Worksheet 12.3 The Lorentz transformation is the same as above. We set the condition $\Delta x' = 0$ in `Eq3`, and solve for Δx in `Eq4`. Substituting `dx` into `Eq1`, we obtain the relation between primed and unprimed frames in `Eq7`.

```
> with(LinearAlgebra):
> gma := 1/sqrt(1 - beta^2):
> L := << gma | -gma*beta | 0 | 0 >, < -gma*beta | gma | 0 | 0 >,
< 0 | 0 | 1 | 0 >, < 0 | 0 | 0 | 1 >>;
```

$$L := \begin{bmatrix} \frac{1}{\sqrt{1-\beta^2}} & -\frac{\beta}{\sqrt{1-\beta^2}} & 0 & 0 \\ -\frac{\beta}{\sqrt{1-\beta^2}} & \frac{1}{\sqrt{1-\beta^2}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

```
> txyz := < c*dt, dx, dy, dz >:
> txyzp := L.txyz:
> txyzp := map(simplify, txyzp):
> Eq1 := dtp = txyzp[1]/c;
```

$$Eq1 := dtp = \frac{c\,dt - \beta\,dx}{\sqrt{1-\beta^2}\,c}$$

```
> Eq2 := dxp = txyzp[2];
```

$$Eq2 := dxp = -\frac{\beta\,c\,dt - dx}{\sqrt{1-\beta^2}}$$

```
> Eq3 := eval(Eq2, dxp=0);
```

$$Eq3 := 0 = -\frac{\beta\,c\,dt - dx}{\sqrt{1-\beta^2}}$$

```
> Eq4 := isolate(Eq3, dx);
```

$$Eq4 := dx = \beta\,c\,dt$$

```
> Eq5 := subs(Eq4, Eq1);
```

$$Eq5 := dtp = \frac{c\,dt - \beta^2\,c\,dt}{\sqrt{1-\beta^2}\,c}$$

```
> Eq6 := isolate(Eq5, dt):
> Eq7 := simplify(Eq6);
```

$$Eq7 := dt = \frac{dtp}{\sqrt{1-\beta^2}}$$

A space–time interval is a four-vector; its scalar product is with itself and therefore is an invariant quantity. If the scalar product of the space–time interval is negative, we define the

proper time τ (always positive) as:

$$c^2 d\tau^2 \equiv ds^2 = c^2 dt^2 - dx^2 - dy^2 - dz^2 = c^2 dt'^2 - dx'^2 - dy'^2 - dz'^2. \quad (12.18)$$

We interpret the proper time as the time read by a clock comoving with a given object, for which spatial components vanish; in the above example of time dilation, $d\tau = dt'$ because $dx' = dy' = dz' = 0$. If we seek to know what a clock reads in frame K', in terms of a clock at rest in frame K, the situation is reversed: finding the primed parameter in terms of unprimed ones, we integrate equation (12.18):

$$\tau_2 - \tau_1 = \int_{t_1}^{t_2} dt \sqrt{1 - \frac{u^2}{c^2}}. \quad (12.19)$$

This integral yields the time interval for a moving clock when the corresponding interval according to a clock at rest is $t_2 - t_1$.

12.1.2 Addition of Velocity

We maintain the definitions of frames K and K' according to the preceding section: for K' moving at velocity u in the x direction, we discuss the velocity addition rule according to relativity. Suppose that an object moves at velocity v' in the x' direction according to an observer in K'. We seek the velocity v_x of this object moving from a point of view of an observer in the K frame.

The infinitesimal separation between two events transforms as

$$\begin{aligned} dt' &= \frac{dt - u dx/c^2}{\sqrt{1 - u^2/c^2}}, \\ dx' &= \frac{dx - u dt}{\sqrt{1 - u^2/c^2}}, \\ dy' &= dy, \\ dz' &= dz. \end{aligned} \quad (12.20)$$

The velocity v'_x according to an observer in the K' frame is

$$v'_x = \frac{dx'}{dt'}.$$

Our objective is to find v_x (unprimed), which is

$$v_x = \frac{dx}{dt},$$

in terms of v'_x (primed) and u.

From these transformations, we write directly

$$v'_x = \frac{dx - u dt}{dt - u dx/c^2}.$$

Isolating dx/dt from this formula, we obtain

$$v_x = \frac{dx}{dt} = \frac{u + v'_x}{1 + uv'_x/c^2}. \tag{12.21}$$

This is the velocity addition rule in relativity.

Worksheet 12.4 In this worksheet, `dtp` and `dxp` denote dt' and dx', respectively; `vxp`, denoting v'_x, is expressed in `Eq1`. In `Eq2` and `Eq3` we isolate dx/dt from v'_x.

```
> with(LinearAlgebra):
> gma := 1/sqrt(1 - beta^2): beta := u/c;
```

$$\beta := \frac{u}{c}$$

```
> L := << gma | -gma*beta | 0 | 0 >, < -gma*beta | gma | 0 | 0 >,
< 0 | 0 | 1 | 0 >, < 0 | 0 | 0 | 1 >>;
```

$$L := \begin{bmatrix} \dfrac{1}{\sqrt{1-\dfrac{u^2}{c^2}}} & -\dfrac{u}{\sqrt{1-\dfrac{u^2}{c^2}}\,c} & 0 & 0 \\ -\dfrac{u}{\sqrt{1-\dfrac{u^2}{c^2}}\,c} & \dfrac{1}{\sqrt{1-\dfrac{u^2}{c^2}}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

```
> txyz := < c*dt, dx, dy, dz >;
```

$$txyz := \begin{bmatrix} c\,dt \\ dx \\ dy \\ dz \end{bmatrix}$$

```
> txyzp := L.txyz:
> txyzp := map(simplify, txyzp);
```

$$txyzp := \begin{bmatrix} -\dfrac{-c^2\,dt + u\,dx}{\sqrt{-\dfrac{-c^2+u^2}{c^2}}\,c} \\ -\dfrac{u\,dt - dx}{\sqrt{-\dfrac{-c^2+u^2}{c^2}}} \\ dy \\ dz \end{bmatrix}$$

```
> dtp := txyzp[1]/c; dxp := txyzp[2];
```

$$dtp := -\frac{-c^2\,dt + u\,dx}{\sqrt{-\dfrac{-c^2+u^2}{c^2}}\,c^2}$$

$$dxp := -\frac{u\,dt - dx}{\sqrt{-\dfrac{-c^2+u^2}{c^2}}}$$

```
> Eq1 := dxp/dtp = vxp;
```

$$Eq1 := \frac{(u\,dt - dx)\,c^2}{-c^2\,dt + u\,dx} = vxp$$

```
> Eq2 := isolate(Eq1, dx);
```

$$Eq2 := dx = \frac{c^2\,dt\,(u + vxp)}{c^2 + vxp\,u}$$

```
> Eq3 := lhs(Eq2/dt) = rhs(Eq2/dt):
> Eq4 := simplify(Eq3);
```

$$Eq4 := \frac{dx}{dt} = \frac{c^2\,(u + vxp)}{c^2 + vxp\,u}$$

12.1.3 Doppler Shift

Consider a plane wave of frequency ω' and wave vector $\mathbf{k}' = (k'_x, k'_y, k'_z)$ in the moving frame K'. This wave is viewed to have a different frequency ω and direction of propagation $\mathbf{k} = (k_x, k_y, k_z)$ according to a stationary observer in the K frame. Such an effect is called the Doppler shift. Based on the fact that frequency and three components of the wave vector form a four-vector, we derive the formula for the Doppler shift from the Lorentz transformation.

If a wave propagates along the x' axis, the transformation is simple. Here we consider a more general situation. Suppose a wave propagates in the plane $x'y'$, making an angle ϕ' with the x' axis. According to an observer in the K frame, the wave appears to make an angle ϕ with the x axis; see Figure 12.1.

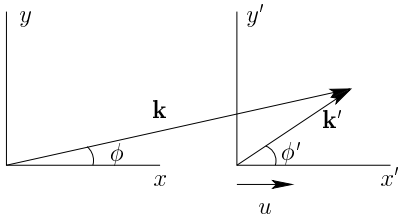


Figure 12.1: Doppler shift.

For an electromagnetic wave, the speed of light is constant; that is,

$$c = \frac{\omega}{k} = \frac{\omega'}{k'}.$$

Assume the magnitude of the wave vector to be k in the K frame; the four-vector is therefore $(k, k\cos\phi, k\sin\phi, 0)$. In the K' frame, the four-vector is $(k', k'\cos\phi', k'\sin\phi', 0)$. We can relate these two sets of four-vectors through the Lorentz transformation:

$$\begin{aligned}\begin{pmatrix} k' \\ k'\cos\phi' \\ k'\sin\phi' \\ 0 \end{pmatrix} &= \begin{pmatrix} \gamma & -\gamma\beta & 0 & 0 \\ -\gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} k \\ k\cos\phi \\ k\sin\phi \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} \gamma k(1-\beta\cos\phi) \\ \gamma k(\cos\phi - \beta) \\ k\sin\phi \\ 0 \end{pmatrix}.\end{aligned} \tag{12.22}$$

Our objective is again to express unprimed parameters in terms of primed parameters. Comparing both sides of the equation, we solve for $\cos\phi$ and k in terms of $\cos\phi'$ and k'. We obtain the frequency (recall that $\omega = ck$ and $\omega' = ck'$) to be

$$\omega = \frac{1+\beta\cos\phi'}{\sqrt{1-\beta^2}}\omega'; \tag{12.23}$$

the angles ϕ and ϕ' are related as

$$\cos\phi = \frac{\cos\phi' + \beta}{1+\beta\cos\phi'}. \tag{12.24}$$

Worksheet 12.5 In this worksheet, the meaning of the symbols is evident; we use `phip` to denote ϕ'. We obtain k and $\cos\phi$ on solving the equations in `Soln1`. Be aware that the order of appearance of quantities in a solution set in Maple is generally unpredictable. After finding k and $\cos\phi$ in `Eq6` and `Eq7`, we discuss two special cases for $\phi = 0$ and $\phi = \pi/2$. Calculations pertaining to the $\phi = 0$ case are from `Eq11` to `Eq14`: we need to find $\cos\phi'$ first, which is `Eq12`, so that we can find k, which is `Eq14`. The calculations for the $\phi = \pi$ case are from `Eq21` to `Eq24`.

```
> with(LinearAlgebra):
> gma := 1/sqrt(1 - beta^2):
> L := << gma | -gma*beta | 0 | 0 >, < -gma*beta | gma | 0 | 0 >,
< 0 | 0 | 1 | 0 >, < 0 | 0 | 0 | 1 >>;
```

$$L := \begin{bmatrix} \dfrac{1}{\sqrt{1-\beta^2}} & -\dfrac{\beta}{\sqrt{1-\beta^2}} & 0 & 0 \\ -\dfrac{\beta}{\sqrt{1-\beta^2}} & \dfrac{1}{\sqrt{1-\beta^2}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

```
> omega := k*c; kx := k*cos(phi); ky := k*sin(phi); kz := 0;
```

$$\omega := k\,c$$
$$kx := k\cos(\phi)$$
$$ky := k\sin(\phi)$$
$$kz := 0$$

```
> wavevec := < omega/c, kx, ky, kz >;
```

$$wavevec := \begin{bmatrix} k \\ k\cos(\phi) \\ k\sin(\phi) \\ 0 \end{bmatrix}$$

```
> wavevecprime := L.wavevec:
> wavevecprime := map(simplify, wavevecprime);
```

$$wavevecprime := \begin{bmatrix} -\dfrac{k\,(-1+\beta\cos(\phi))}{\sqrt{1-\beta^2}} \\ -\dfrac{k\,(\beta-\cos(\phi))}{\sqrt{1-\beta^2}} \\ k\sin(\phi) \\ 0 \end{bmatrix}$$

```
> Eq1 := kp = wavevecprime[1];
```

$$Eq1 := kp = -\frac{k\,(-1+\beta\cos(\phi))}{\sqrt{1-\beta^2}}$$

```
> Eq2 := kp*cos(phip) = wavevecprime[2];
```

$$Eq2 := kp\cos(phip) = -\frac{k\,(\beta-\cos(\phi))}{\sqrt{1-\beta^2}}$$

```
> Eq3 := kp*sin(phip) = wavevecprime[3];
```

$$Eq3 := kp\sin(phip) = k\sin(\phi)$$

```
> Soln1 := solve({Eq1, Eq2}, {k, cos(phi)}); # be aware of order
```

$$Soln1 := \left\{ k = -\frac{kp\,\sqrt{-(\beta-1)\,(\beta+1)}\,(1+\beta\cos(phip))}{-1+\beta^2},\ \cos(\phi) = \frac{\cos(phip)+\beta}{1+\beta\cos(phip)} \right\}$$

```
> Eq6 := simplify(Soln1[1]); # for k
```

$$Eq6 := k = \frac{(1+\beta\cos(phip))\,kp}{\sqrt{1-\beta^2}}$$

```
> Eq7 := simplify(Soln1[2]); # for cos(phi)
```

$$Eq7 := \cos(\phi) = \frac{\cos(phip)+\beta}{1+\beta\cos(phip)}$$

```
> Eq11 := eval(Eq7, phi=0);
```

$$Eq11 := 1 = \frac{\cos(phip) + \beta}{1 + \beta\cos(phip)}$$

```
> Eq12 := isolate(Eq11, cos(phip));
```

$$Eq12 := \cos(phip) = 1$$

```
> Eq13 := subs(Eq12, Eq6):
> Eq14 := simplify(Eq13);
```

$$Eq14 := k = \frac{(\beta + 1)\, kp}{\sqrt{1 - \beta^2}}$$

```
> Eq21 := eval(Eq7, phi=Pi/2);
```

$$Eq21 := 0 = \frac{\cos(phip) + \beta}{1 + \beta\cos(phip)}$$

```
> Eq22 := isolate(Eq21, cos(phip));
```

$$Eq22 := \cos(phip) = -\beta$$

```
> Eq23 := subs(Eq22, Eq6):
> Eq24 := simplify(Eq23);
```

$$Eq24 := k = kp\,\sqrt{1 - \beta^2}$$

We discuss special situations. If the wave propagates in the $+x$ direction, then $\phi = 0$; from Figure 12.1 we see that $\phi' = 0$ also. We verify this result mathematically in the above Maple worksheet. With a supplementary manual arrangement, we obtain

$$\omega = \sqrt{\frac{1+\beta}{1-\beta}}. \tag{12.25}$$

This equation corresponds to the situation when a moving source directly approaches a stationary observer. We can also obtain a formula for a wave propagating in the $-x$ direction. In this case, $\phi = \phi' = \pi$, so

$$\omega = \sqrt{\frac{1-\beta}{1+\beta}}. \tag{12.26}$$

This equation corresponds to a moving source that directly recedes from a stationary observer.

A transverse Doppler shift occurs when the wave is received perpendicularly. This condition signifies that $\phi = \pi/2$ (be aware that it is the unprimed ϕ); hence the wave propagates perpendicularly in the K frame, but there is still a shift in frequency. We solve for ϕ' first, which is

$$\cos\phi = \frac{\pi}{2}, \quad \cos\phi' = -\beta;$$

substituting this condition into our general formula in equation (12.23), we obtain

$$\omega = \sqrt{1-\beta^2}\omega'. \tag{12.27}$$

This result implies a decrease in frequency.

In many textbooks, the inverse Lorentz transformation is introduced on observing that K is considered to move at $-u$ away from K'; unprimed parameters are hence readily expressed in terms of primed ones. We avoid this argument because it might generate confusion about who is moving. We only apply the transformation properties to obtain the primed four-vectors, and employ Maple to solve directly for unprimed quantities.

12.2 Relativistic Kinematics and Dynamics

Newton's second law is

$$F = \frac{d}{dt}(mv). \tag{12.28}$$

This equation is not invariant under the Lorentz transformation if we consider the mass m to be constant (independent of velocity v). If our concern is only to solve problems, to make Newtonian mechanics consistent with relativity, we simply multiply the mass by a factor γ,

$$m \to \frac{m_0}{\sqrt{1-v^2/c^2}}, \tag{12.29}$$

so that equation (12.28) becomes invariant under the Lorentz transformation; the quantity m_0 signifies the rest mass.

Just as Newton's second law must be modified to conform to the Lorentz transformation, definitions of energy and momentum must be modified accordingly. The relativistic momentum is defined as

$$\mathbf{p} = \frac{m_0\mathbf{u}}{\sqrt{1-u^2/c^2}}; \tag{12.30}$$

relativistic energy is

$$E = \frac{m_0c^2}{\sqrt{1-u^2/c^2}}. \tag{12.31}$$

Together they form a four-vector

$$p^\mu = (E/c, p_x, p_y, p_z). \tag{12.32}$$

Because the scalar product of the energy-momentum four-vector with itself is an invariant,

$$p^\mu p_\mu = -\left(\frac{E}{c}\right)^2 + \mathbf{p}\cdot\mathbf{p} = -m_0^2c^2, \tag{12.33}$$

we acquire an important relation between energy and momentum:

$$E^2 = (m_0c^2)^2 + (pc)^2. \tag{12.34}$$

Consider an arbitrary collision process; if there is no external force, the sum of the energy-momentum four-vector in each component is conserved:

$$\sum_i E_{ia} = \sum_j E_{jb}, \tag{12.35}$$

$$\sum_i \mathbf{p}_{ia} = \sum_j \mathbf{p}_{jb}. \tag{12.36}$$

Indices a and b pertain to particles after and before the collision, respectively.

Example 12.1 Two particles with rest masses m_1 and m_2 move in one dimension. Particle 1 has initial velocity u_{1b}, and particle 2 is at rest. Assuming the collision to be elastic – under which condition the rest masses are unchanged, find the final velocity of particle 1 after the collision.

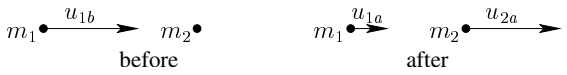


Figure 12.2: One-dimensional relativistic collision problem.

Solution Both energy and momentum are conserved:

$$E_{1a} + E_{2a} = E_{1b} + E_{2b}, \tag{12.37}$$

and

$$p_{1a} + p_{2a} = p_{1b} + p_{2b}, \tag{12.38}$$

with E_{1b} as the energy of particle 1 before the collision and E_{1a} as its energy afterwards, and analogously, E_{2b} and E_{2a} for particle 2. Using the relativistic energy and momentum, we have

$$\frac{m_1c^2}{\sqrt{1-u_{1a}^2/c^2}} + \frac{m_2c^2}{\sqrt{1-u_{2a}^2/c^2}} = \frac{m_1c^2}{\sqrt{1-u_{1b}^2/c^2}} + m_2c^2, \tag{12.39}$$

and

$$\frac{m_1u_{1a}}{\sqrt{1-u_{1a}^2/c^2}} + \frac{m_2u_{2a}}{\sqrt{1-u_{2a}^2/c^2}} = \frac{m_1u_{1b}}{\sqrt{1-u_{1b}^2/c^2}}. \tag{12.40}$$

Solving the above two equations with two unknowns u_{1a} and u_{2a}, we obtain the final velocity of particle m_1:

$$u_{1a} = \frac{m_1^2 - m_2^2}{m_1^2 + m_2^2 + 2m_1 m_2\sqrt{1 - u_{1b}^2/c^2}} u_{1b}. \tag{12.41}$$

Worksheet 12.6 The symbols are self-evident. We evaluate the limit $c \to \infty$ at the end for the classical formula. The order of appearance of solutions in a set is unpredictable; for this reason be aware of the selection of `Soln1[2,2]` as `u1a` in the `limit`.

```
> Eq1 := m1/sqrt(1-u1a^2/c^2) + m2/sqrt(1-u2a^2/c^2) =
> m1/sqrt(1-u1b^2/c^2) + m2;
```

$$Eq1 := \frac{m1}{\sqrt{1 - \frac{u1a^2}{c^2}}} + \frac{m2}{\sqrt{1 - \frac{u2a^2}{c^2}}} = \frac{m1}{\sqrt{1 - \frac{u1b^2}{c^2}}} + m2$$

```
> Eq2 := m1*u1a/sqrt(1-u1a^2/c^2) + m2*u2a/sqrt(1-u2a^2/c^2) =
> m1*u1b/sqrt(1-u1b^2/c^2);
```

$$Eq2 := \frac{m1\ u1a}{\sqrt{1 - \frac{u1a^2}{c^2}}} + \frac{m2\ u2a}{\sqrt{1 - \frac{u2a^2}{c^2}}} = \frac{m1\ u1b}{\sqrt{1 - \frac{u1b^2}{c^2}}}$$

```
> Soln1 := solve({Eq1, Eq2}, {u1a, u2a});
```

$$Soln1 := \{u2a = 0,\ u1a = u1b\}, \left\{ u2a = 2\ m1\ u1b \right.$$

$$\left(m2\ c^2 - m2\ u1b^2 + \sqrt{\frac{(c - u1b)\,(c + u1b)}{c^2}}\ c^2\ m1 \right) \Big/ \Bigg(\left(2\ c^2\ m2\ m1 \sqrt{\frac{(c - u1b)\,(c + u1b)}{c^2}} + c^2\ m2^2 + c^2\ m1^2 - m2^2\ u1b^2 + m1^2\ u1b^2 \right) \sqrt{\frac{(c - u1b)\,(c + u1b)}{c^2}} \Bigg),\ u1a = \left. \frac{u1b\,(m1^2 - m2^2)}{2\ m2\ m1 \sqrt{\frac{(c - u1b)\,(c + u1b)}{c^2}} + m2^2 + m1^2} \right\}$$

```
> limit(Soln1[2,2], c=infinity); #select the right solution
```

$$u1a = \frac{u1b\ m1 - u1b\ m2}{m2 + m1}$$

We see that in the nonrelativistic limit, for which $c = \infty$, u_{1a} reduces to the classical formula in Section 1.2.

Although Newton's second law in the form $F = ma$ is invalid at a high speed, modifying the mass with a correction factor γ is all that one needs to solve a problem in dynamics. Namely, we have

$$\mathbf{F} = \frac{d}{dt}\mathbf{p}, \tag{12.42}$$

provided that we use the relativistic momentum defined in equation (12.30). We offer an example as an illustration.

Example 12.2 For a particle subject to a constant force F, find its position as a function of time.

Solution From equation (12.42), we can write directly

$$F = \frac{d}{dt}\frac{mu(t)}{\sqrt{1-[u(t)/c]^2}}, \tag{12.43}$$

where $u(t) = \dot{x}(t)$. Maple can solve this differential equation for $x(t)$ – try it. However, we perform a more detailed analysis to gain an insight.

Momentum is the integral of force with respect to time, and for a constant force, such a calculation is easy:

$$\frac{mu}{\sqrt{1-u^2/c^2}} = Ft, \quad \text{supposing } u(0) = 0.$$

We next solve for u,

$$u = \frac{Fct}{\sqrt{(Ft)^2 + (mc)^2}}. \tag{12.44}$$

Supposing that $x(0) = 0$, we integrate u to obtain

$$x = \frac{c}{F}\left[\sqrt{(mc)^2 + (Ft)^2} - mc\right]. \tag{12.45}$$

For comparison, according to Newtonian mechanics, the position is expected to be

$$x = \frac{1}{2}at^2 = \frac{1}{2}\frac{F}{m}t^2.$$

Worksheet 12.7 The integrals are evaluated with Maple. The symbols `pos` and `poscl` denote positions according to relativity and classical mechanics, respectively. To make the plot, we assign unit values to `F`, `m` and `c`.

```
> p := m*u/sqrt(1-u^2/c^2);
```

$$p := \frac{m\,u}{\sqrt{1-\frac{u^2}{c^2}}}$$

```
> Eq1 := p = F*tp;
```

$$Eq1 := \frac{m\,u}{\sqrt{1-\frac{u^2}{c^2}}} = F\,tp$$

```
> Eq2 := solve(Eq1,u);
```

$$Eq2 := \frac{F\,tp\,c}{\sqrt{F^2\,tp^2+c^2\,m^2}}, -\frac{F\,tp\,c}{\sqrt{F^2\,tp^2+c^2\,m^2}}$$

```
> pos := int(Eq2[1], tp=0..t);
```

$$pos := \frac{c\,(\sqrt{F^2\,t^2+c^2\,m^2}-\sqrt{c^2\,m^2})}{F}$$

```
> poscl := 1/2*(F/m)*t^2;
```

$$poscl := \frac{F\,t^2}{2\,m}$$

```
> c:=1; F:=1; m:=1;
```

$$c := 1$$
$$F := 1$$
$$m := 1$$

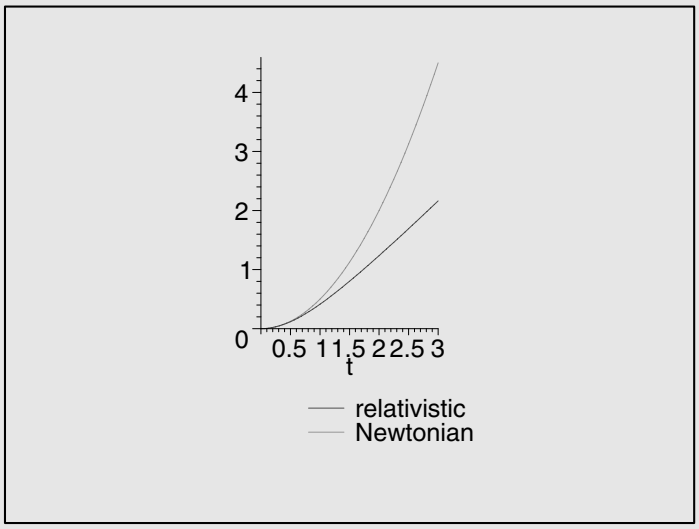
```
> pos;
```

$$\sqrt{t^2+1}-1$$

```
> poscl;
```

$$\frac{t^2}{2}$$

```
> plot([pos, poscl], t=0..3, scaling=constrained,
> legend=["relativistic", "Newtonian"]);
```



In the graph of x as a function of time, the slope corresponds to the velocity. We observe that the curve based on relativity is a hyperbola, with a slope approaching the speed of light, while the curve based on Newtonian mechanics is a parabola, with a slope approaching infinity.

Let us explore an interesting aspect of this motion. If a rocket has engines that give it a constant acceleration of one earth gravity, g, it will not cause discomfort for the astronauts on board. Coincidentally, g almost exactly equals one light year (ly) per year (yr) squared – a reader can verify that $g = 9.8$ m s$^{-2} = 1.03$ ly yr^{-2}. Using $g = 1$ ly yr^{-2} and $c = 1$ ly yr^{-1}, and year to measure t, equations (12.44) and (12.45) become

$$u = \frac{t}{\sqrt{t^2 + 1}},$$

and

$$x = \sqrt{1 + t^2} - 1,$$

where x is measured in light years. Suppose that this rocket is sent to travel from the earth to the center of the galaxy at 30 000 light years away, and it accelerates for half the trip then decelerates for the remaining half. Maintaining an acceleration of 1 ly yr^{-2}, the rocket attains a speed of $u = 1/\sqrt{2}\ c = 0.71\ c$ after one year, $u = 2/\sqrt{5}\ c = 0.89\ c$ after two years, and $u = 3/\sqrt{10}\ c = 0.95\ c$ after three years. The midway time t_h can be obtained from

$$15\,000 = \sqrt{1 + t_h^2} - 1,$$

which gives $t_h = 15\,001$ yr; this value is understandable because within years, the speed of the rocket is essentially the speed of light; for a large t, $x \simeq t$. So far we have been using the

coordinate and time based on earth. The astronauts, however, read the proper time τ_h of their world line, see equation (12.19), which is

$$\tau_h = \int_0^{t_h} \sqrt{1 - \frac{u^2}{c^2}}\, dt = \int_0^{15001} \sqrt{1 - \frac{t^2}{t^2+1}}\, dt = 10.3 \text{ (yr)}.$$

The calculation for the deceleration is identical to that of the acceleration, so we simply double t_h and τ_h for the entire journey. We conclude that while $30\,002$ years will elapse for the mission control on the ground, the astronauts on board will age by only 20.6 years!

12.3 Transformations of Electromagnetic Fields

As described in Section 8.1, a charge in the presence of both electric and magnetic fields experiences the Lorentz force:

$$\frac{d\mathbf{p}}{dt} = q[\mathbf{E} + (\mathbf{v} \times \mathbf{B})]. \tag{12.46}$$

We can always discover a frame which comoves with the charge at $\mathbf{u} = \mathbf{v}$, so that in such a frame there is no magnetic force. This property implies that a magnetic field is simply an electric field in motion from the point of view of relativity. Conversely, because there is no frame that is superior to another, $\mathbf{E}$ and $\mathbf{B}$ have no independent existence: a purely electric or magnetic field in one frame appears as a mixture of electric and magnetic fields in another frame.

The transformation of an electromagnetic field involves a tensor of second rank. By definition, a four-vector implies four components that transform according to the Lorentz transformation:

$$\mathbf{a}' = \mathbf{L}\mathbf{a}. \tag{12.47}$$

To extend this concept, we define a four-tensor of second rank to be sixteen quantities $t^{\alpha\beta}$ in a 4×4 matrix, which transforms as

$$\mathbf{t}' = \mathbf{L}\mathbf{t}\tilde{\mathbf{L}}; \tag{12.48}$$

this is a similarity transformation in matrix algebra.

The components of electric and magnetic fields (in total six elements) form an antisymmetric field tensor $\mathbf{T}$:

$$\begin{pmatrix} 0 & E_x/c & E_y/c & E_z/c \\ -E_x/c & 0 & B_z & -B_y \\ -E_y/c & -B_z & 0 & B_x \\ -E_z/c & B_y & -B_x & 0 \end{pmatrix}. \tag{12.49}$$

Using the transformation property of a tensor, we derive the formula for an electromagnetic field viewed by a moving observer:

$$\mathbf{T}' = \mathbf{L}\mathbf{T}\tilde{\mathbf{L}}. \tag{12.50}$$

Performing the matrix multiplications, we obtain the transformation for an electromagnetic field:

$$\begin{array}{ll} E'_x = E_x, & B'_x = B_x, \\ E'_y = \gamma(E_y - vB_z), & B'_y = \gamma\left(B_y + \dfrac{v}{c^2}E_z\right), \\ E'_z = \gamma(E_z + vB_y), & B'_z = \gamma\left(B_z - \dfrac{v}{c^2}E_y\right). \end{array} \tag{12.51}$$

Worksheet 12.8 Matrix multiplication is a simple task for Maple; the meaning of this worksheet is apparent.

```
> with(LinearAlgebra):
> T := << 0 | Ex/c | Ey/c | Ez/c >, <-Ex/c | 0 | Bz | -By >,
> < -Ey/c | -Bz | 0 | Bx >, < -Ez/c | By | -Bx | 0 >>;
```

$$T := \begin{bmatrix} 0 & \frac{Ex}{c} & \frac{Ey}{c} & \frac{Ez}{c} \\ -\frac{Ex}{c} & 0 & Bz & -By \\ -\frac{Ey}{c} & -Bz & 0 & Bx \\ -\frac{Ez}{c} & By & -Bx & 0 \end{bmatrix}$$

```
> gma:=1/sqrt(1-beta^2);
```

$$gma := \frac{1}{\sqrt{1-\beta^2}}$$

```
> L := << gma | -gma*beta | 0 | 0 >, < -gma*beta | gma | 0 | 0 >,
> < 0 | 0 | 1 | 0 >, < 0 | 0 | 0 | 1 >>;
```

$$L := \begin{bmatrix} \frac{1}{\sqrt{1-\beta^2}} & -\frac{\beta}{\sqrt{1-\beta^2}} & 0 & 0 \\ -\frac{\beta}{\sqrt{1-\beta^2}} & \frac{1}{\sqrt{1-\beta^2}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

```
> Tp:=L.T.Transpose(L):
```

```
> map(simplify, Tp);
```

$$\begin{bmatrix} 0 & \frac{Ex}{c} & -\frac{-Ey+\beta\,Bz\,c}{\sqrt{1-\beta^2}\,c} & \frac{Ez+\beta\,By\,c}{\sqrt{1-\beta^2}\,c} \\ -\frac{Ex}{c} & 0 & \frac{-\beta\,Ey+Bz\,c}{\sqrt{1-\beta^2}\,c} & -\frac{\beta\,Ez+By\,c}{\sqrt{1-\beta^2}\,c} \\ \frac{-Ey+\beta\,Bz\,c}{\sqrt{1-\beta^2}\,c} & -\frac{-\beta\,Ey+Bz\,c}{\sqrt{1-\beta^2}\,c} & 0 & Bx \\ -\frac{Ez+\beta\,By\,c}{\sqrt{1-\beta^2}\,c} & \frac{\beta\,Ez+By\,c}{\sqrt{1-\beta^2}\,c} & -Bx & 0 \end{bmatrix}$$

Exercises

1. For a situation in which a particle moves in a plane with both v'_x and v'_y nonvanishing (see Figure 12.3), verify the velocity addition rule:

$$v_x = \frac{u + v'_x}{1 + uv'_x/c^2}, \quad v_y = \frac{\sqrt{1-u^2/c^2}\,v'_y}{1 + uv'_x/c^2}. \tag{12.52}$$

Using the definitions of $v'_x \equiv v'\cos\phi'$, $v'_y \equiv v'\sin\phi'$, $v_x \equiv v\cos\phi$ and $v_y \equiv v\sin\phi$,

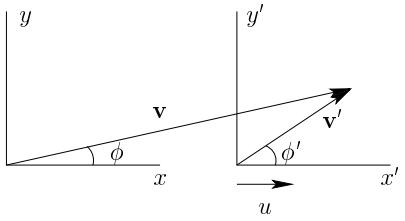


Figure 12.3: Addition of velocities.

verify that

$$v = \frac{\sqrt{u^2 + v'^2 + 2uv'\cos\phi' - (uv'\sin\phi'/c)^2}}{1 + uv'\cos\phi'/c^2}, \tag{12.53}$$

where ϕ and ϕ' are related as

$$\tan\phi = \frac{v'\sin\phi'\sqrt{1-u^2/c^2}}{u + v'\cos\phi'}. \tag{12.54}$$

2. Derive the formula for the Doppler shift for a situation in which, in contrast to the example in the text, we consider a stationary source in K that emits a wave of frequency ω; we seek ω' viewed by a moving observer in K'.

Hint: unlike a sound wave, the formula for the Doppler shift of an electromagnetic wave is independent of whether a source or a receiver is moving.

3. The relativistic kinetic energy is defined as the total energy minus the rest energy:

$$E_{\text{kin}} = \frac{m_0 c^2}{\sqrt{1 - u^2/c^2}} - m_0 c^2. \tag{12.55}$$

(a) Expand the relativistic kinetic energy in the powers of u to verify that

$$E_{\text{kin}} = \frac{1}{2} m u^2 + \frac{3}{8} \frac{m u^4}{c^2} + \ldots. \tag{12.56}$$

The leading term reproduces the classical formula.

(b) According to the above formula, find the speed when the kinetic energies determined classically and relativistically differ by 1%.

(c) In terms of momentum, the relativistic kinetic energy is

$$E_{\text{kin}} = \sqrt{p^2 c^2 + m_0^2 c^4} - m c^2. \tag{12.57}$$

Expand the kinetic energy in powers of p to verify that

$$E_{\text{kin}} = \frac{p^2}{2 m_0} - \frac{p^4}{8 m_0^3 c^2} + \ldots. \tag{12.58}$$

Again the leading term is the classical formula; the lowest-order relativistic correction to the Hamiltonian is therefore

$$\Delta H_{\text{rel}} = -\left(\frac{1}{8 m_0^3 c^2} \right) p^4. \tag{12.59}$$

This term is useful in calculating relativistic correction in quantum mechanics.

4. Two particles, each having rest mass m_0, collide head on at $\frac{3}{5}\, c$; after the collision they stick together. What is the mass of the composite particle?

5. The Lagrangian for a relativistic particle is

$$L = -m c^2 \sqrt{1 - \frac{u^2}{c^2}} - V. \tag{12.60}$$

Suppose a particle is influenced by a constant force F, so that $V = Fx$. Employing the Euler–Lagrange equation, derive the equation of motion using the method discussed in Chapter 3, and solve the differential equation. One expects the result to be a hyperbola, identical to equation (12.45).

6. The twin paradox involves an astronaut taking a trip at a relativistic speed to a planet then returning to the earth; though much has been written about it, few mention the acceleration required to attain the relativistic speed, say v, from rest.[1] Assuming a constant acceleration a in the astronaut's frame, we rewrite equation (12.44) as

$$u = \frac{at}{\sqrt{(at/c)^2 + 1}}, \tag{12.61}$$

which is the speed of the rocket according to an observer on the earth. Without ignoring the accelerating process, let a journey consist of four sections, each consuming the same amount of time: (1) acceleration for half of the trip until the rocket reaches a speed v; (2) deceleration for the remaining half so that the rocket stops on the planet; (3) acceleration for half of the return trip until the rocket reaches a speed v; (4) deceleration for the remaining half so that the rocket stops on earth.

(a) From equation (12.61), show that the lapse of proper time for an observer on earth is

$$T = \frac{v}{a} \frac{1}{\sqrt{1 - v^2/c^2}}. \tag{12.62}$$

(b) From equation (12.19), show that the lapse of proper time for the astronaut is

$$\tau = \int_0^T \sqrt{1 - \frac{u^2}{c^2}} = \frac{c}{a} \ln \sqrt{\frac{c+v}{c-v}}, \tag{12.63}$$

where T is in equation (12.62); this result can be equivalently expressed as

$$\tau = \frac{c}{a} \tanh^{-1} \frac{v}{c}. \tag{12.63$'$}$$

Make a plot of T and τ versus v, and one should observe that

$$T > \tau. \tag{12.64}$$

7. (a) Verify that $\mathbf{E} \cdot \mathbf{B}$ is an invariant quantity under the Lorentz transformation; that is

$$\mathbf{E}' \cdot \mathbf{B}' = \mathbf{E} \cdot \mathbf{B}.$$

(b) Verify also that a quantity $\mathbf{B} \cdot \mathbf{B} - \mathbf{E} \cdot \mathbf{E}$ is invariant under the Lorentz transformation.

8. In Section 8.1, we calculate the motion of a charged particle in the magnetic field. Although the Lorentz force law is correct, the famous $F = ma$ is not in relativity. There is a simple remedy: we write $F = \frac{dp}{dt}$, and p is modified by a Lorentz factor γ, thus the equation of motion becomes

$$\frac{d}{dt}\mathbf{p} = \frac{d}{dt}(\gamma m \mathbf{v}) = q\mathbf{v} \times \mathbf{B}, \tag{12.65}$$

[1] Acceleration in special relativity is treated in C. W. Misner, K. S. Thorne, and J. A. Wheeler, *Gravitation*, San Francisco: Freeman, 1973, Chapter 6; our calculation is essentially the answer to exercise 6.3 on p. 167 of that book.

where $\gamma = 1/\sqrt{1 - v^2/c^2}$. Suppose we have a constant magnetic field B_z along the z axis, and a particle with initial velocity v_{0y} in the y direction moves on the xy plane. Because the magnetic force does no work, total energy is conserved, and γ is constant, as well as the magnitude of the velocity.[2] We obtain the equations of motion in components:

$$\gamma m\dot{v}_x = qv_yB_z, \qquad \gamma m\ddot{x} = q\dot{y}B_z, \tag{12.66a}$$

$$\gamma m\dot{v}_y = -qv_xB_z, \quad \gamma m\ddot{y} = -q\dot{x}B_z. \tag{12.66b}$$

Solve these coupled differential equations, assuming $x(0) = 0$ and $y(0) = 0$, to verify that

$$x = \frac{v_{0y}}{\omega}[1 - \cos(\omega t)], \quad y = \frac{v_{0y}}{\omega}\sin(\omega t), \tag{12.67}$$

where

$$\omega = \frac{eB_z}{\gamma m}. \tag{12.68}$$

Notice a γ in the denominator, which differs from the cyclotron frequency in equation (8.5). Substitute numerical values to make a parametric plot of the solutions, and observe that the particle undergoes circular motion at a radius v_{0y}/ω.

[2] The magnitude of the velocity, $v = \sqrt{v_x^2 + v_y^2}$, is constant, but not $\mathbf{v}$ because v_x and v_y are functions of time.

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13 Quantum Phenomena

In this chapter we introduce the experimental details of quantum behavior and their theoretical interpretation. Knowledge of quantum phenomena is required for the four subsequent chapters on quantum mechanics and quantum statistics. We also present Bohr's model for the hydrogen atom, and the statistical approach of paramagnetism, which are two important applications of the old quantum theory.

13.1 Blackbody Radiation

Any object with a temperature above absolute zero emits thermal radiation. In the late nineteenth century, physicists had an active interest in measuring the spectrum of thermal radiation from a blackbody, which is an ideal object, at a particular temperature T that absorbs all radiation incident upon it and that is in equilibrium with radiation. Quantitatively, one measures the energy emitted per unit time per unit area of the surface in an interval of frequency between ν and $\nu + d\nu$; this quantity is called spectral radiancy, $R_T(\nu)d\nu$.

From the spectral radiancy $R_T(\nu)d\nu$ for various temperatures, two empirical laws are observed for a blackbody. First, the frequency at which the curve reaches a maximum ν_{max} is proportional to the temperature,

$$\nu_{\text{max}} \propto T; \tag{13.1}$$

this is Wien's displacement law.

Second, the total flux of energy, which is the integral of spectral radiancy over the entire range of frequency,

$$R_T = \int_0^\infty R_T(\nu)d\nu, \tag{13.2}$$

is proportional to the fourth power of the temperature,

$$R_T = \sigma T^4; \tag{13.3}$$

this is the Stefan–Boltzmann law, where the proportionality constant σ is known as the Stefan–Boltzmann constant, with an experimental value of 5.67×10^{-8} W m^{-2} K^{-4}.

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Two attempts to apply classical physics to the explanation of the spectral radiancy $R_T(\nu)d\nu$ from a blackbody have yielded contradictory results: the Rayleigh–Jeans law and Wien's law. The former accounted for experiments in the regime of long wavelength, and the latter for short wavelength; neither is satisfactory for wavelengths over the entire range.

In 1900 Planck successfully derived a formula to describe the curve $R_T(\nu)d\nu$. The fundamental difference between Planck's approach and the classical derivations is that Planck made an assumption that energy can only assume discrete values,

$$\varepsilon = 0, \Delta\varepsilon, 2\Delta\varepsilon, 3\Delta\varepsilon, 4\Delta\varepsilon, \ldots, \tag{13.4}$$

where

$$\Delta\varepsilon = h\nu. \tag{13.5}$$

The newly introduced constant h is named in honor of Planck.

Among the different ways of deriving Planck's formula for the blackbody spectrum, in Chapter 17 we employ the method of quantum statistics; here we preview the result:

$$R_T(\nu)d\nu = \frac{2\pi h}{c^2}\frac{\nu^3}{e^{h\nu/kT}-1}d\nu. \tag{13.6}$$

Because our concern is radiation from a cavity, we prefer to use the energy density instead of the energy flux. In gas kinematics, the rate of effusion can be calculated from the bombardment of particles on an orifice in the wall of an oven. For photons, the energy density and energy flux are related by a factor of $c/4$,

$$R_T(\nu) = \frac{c}{4}\rho_T(\nu). \tag{13.7}$$

We offer no proof of this result; it is available in the relevant literature.[1]

Planck's formula incorporates the Rayleigh–Jeans law, which is the limit $h\nu/kT \ll 1$, and Wien's formula, which is the limit $h\nu/kT \gg 1$; see one of the exercises at the end of the chapter. It also provides a theoretical basis for those empirical laws. Wien's displacement law is readily derived: differentiating Planck's formula with respect to the frequency and setting the derivative equal to zero, we solve for that frequency corresponding to the maximum of the distribution:

$$\frac{d}{d\nu}R_T(\nu) = 0, \quad \frac{3\nu^2}{e^{h\nu/kT}-1} = \frac{h}{kT}\frac{\nu^3 e^{h\nu/kT}}{(e^{h\nu/kT}-1)^2}. \tag{13.8}$$

We obtain a transcendental equation; apart from a numerical solution, plotting two curves of both sides of the equation and finding their intersections is the graphical method of obtaining the same result. The nontrivial solution is approximately

$$\nu_{\text{max}} = 2.82\frac{kT}{h}. \tag{13.9}$$

[1] Feynman 1965, vol. 1, p. 45-9; Pathria 1996, p. 137ff.

This result provides a rule of thumb: the maximum of the spectral distribution is near the frequency corresponding to an energy of about $3kT$.

The Stefan–Boltzmann law can be obtained as

$$\int_0^\infty \frac{2\pi h}{c^2}\frac{\nu^3}{e^{h\nu/kT}-1}d\nu = \frac{2\pi^5 k^4 T^4}{15h^3c^2}, \tag{13.10}$$

where the Stefan–Boltzmann constant is identified as

$$\sigma = \frac{2\pi^5 k^4}{15h^3c^2}. \tag{13.11}$$

Worksheet 13.1 The meaning of the symbols should be easy to understand. Maple directly performs these calculations, including solving the transcendental equation. We plot the spectral distributions of a blackbody at three temperatures.

```
> assume(c>0, k>0, h>0, T>0):
> R := 2*Pi*h*nu^3/(c^2*(exp(h*nu/(k*T))-1));
```

$$R := \frac{2\,\pi\,h\,\nu^3}{c^2\,(e^{(\frac{h\,\nu}{k\,T})}-1)}$$

```
> Rint := int(R, nu=0..infinity);
```

$$Rint := \frac{2\,\pi^5\,k^4\,T^4}{15\,h^3\,c^2}$$

```
> sigma := Rint/T^4;
```

$$\sigma := \frac{2\,\pi^5\,k^4}{15\,h^3\,c^2}$$

```
> Eq1 := diff(R, nu) = 0;
```

$$Eq1 := \frac{6\,\pi\,h\,\nu^2}{c^2\,(e^{(\frac{h\,\nu}{k\,T})}-1)} - \frac{2\,\pi\,h^2\,\nu^3\,e^{(\frac{h\,\nu}{k\,T})}}{c^2\,(e^{(\frac{h\,\nu}{k\,T})}-1)^2\,k\,T} = 0$$

```
> Soln1 := solve(Eq1, nu);
```

$$Soln1 := \frac{k\,T\,(\mathrm{LambertW}(-3\,e^{(-3)})+3)}{h},\ 0$$

```
> Soln2 := evalf(Soln1);
```

$$Soln2 := \frac{2.821439372\,k\,T}{h},\ 0.$$

```
> R1000 := eval(R, {c=2.998e8, k=1.38e-23, h=6.626e-34, T=1000});
```

$$R1000 := \frac{0.1474409669\,10^{-49}\,\pi\,\nu^3}{e^{(0.4801449275\,10^{-13}\,\nu)}-1}$$

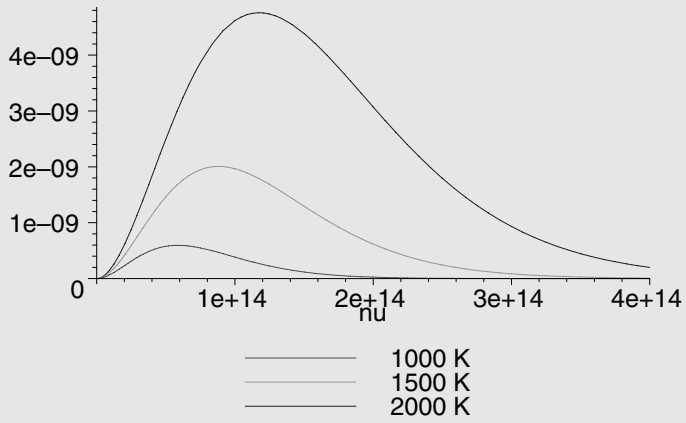
```
> R1500 := eval(R, {c=2.998e8, k=1.38e-23, h=6.626e-34, T=1500});
```

$$R1500 := \frac{0.1474409669\,10^{-49}\,\pi\,\nu^3}{e^{(0.3200966183\,10^{-13}\,\nu)}-1}$$

```
> R2000 := eval(R, {c=2.998e8, k=1.38e-23, h=6.626e-34, T=2000});
```

$$R2000 := \frac{0.1474409669\,10^{-49}\,\pi\,\nu^3}{e^{(0.2400724638\,10^{-13}\,\nu)} - 1}$$

```
> plot([R1000, R1500, R2000], nu=0..4e14, legend=["1000 K",
> "1500 K", "2000 K"]);
```



We mention that equation (13.8) is subject to numerical solution, which is basically a process of trial and error. Scrutinizing the Maple output, the solution of equation (13.8) is, however, expressed as a "known function" – `LambertW`. In the early 1980s, Maple developers included the Lambert W function in the package,[2] which is the function that solves the equation

$$W(x)e^{W(x)} = x. \tag{13.12}$$

This definition enables one to write Wien's displacement law as

$$\nu_{\max} = \left[W(-3e^{-3}) + 3\right] \frac{kT}{h}. \tag{13.13}$$

The Lambert function is managed symbolically in computer algebra like trigonometric, exponential or Bessel functions, which admit integration and differentiation explicitly; it thus can be expanded in an infinite series:

$$W(x) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1} n^{n-2}}{(n-1)!} x^n = x - x^2 + \frac{3}{2}x^3 - \frac{8}{3}x^4 + \frac{125}{24}x^5 - \frac{54}{5}x^6 + \ldots. \tag{13.14}$$

[2]For more applications of this function, see S. R. Valluri, D. J. Jeffrey, and R. M. Corless, "Some applications of the Lambert *W* function to physics," *Canadian Journal of Physics*, **78**, 823–831 (2000).

In contrast to a numerical solver such as the Newton–Raphson method or similar, the above expansion facilitates the most rapid and accurate algorithm in order to evaluate a numerical value to an arbitrary precision. Another application of the Lambert function is the range of projectile motion with air resistance, see one of the exercises at the end of the chapter.

13.2 Photoelectric and Compton Effects

The photoelectric effect is another experiment from the late nineteenth century for which classical theory fails to provide an explanation. When monochromatic light falls on a metallic plate, electrons are ejected: these are called photoelectrons. According to experiment, the maximum kinetic energy of the photoelectron is proportional to the frequency of the light, and there is a definite threshold of frequency, ν_0, below which no photoelectron is emitted.

Einstein proposed that light comprises parcels of energy, called light quanta; each light quantum contains energy E proportional to its frequency,

$$E = h\nu, \tag{13.15}$$

with the Planck constant as a constant of proportionality. In a photoelectric experiment, the energy of a light quantum is acquired by an electron. Using this theory, Einstein successfully explained the photoelectric effect. To escape from a metal, an electron must overcome the energy that binds the electron inside the metal, for which the corresponding energy is called the work function, denoted by w. The remaining energy becomes the kinetic energy of the electron; therefore, the kinetic energy of the electron is proportional to the frequency of the incident radiation. The work function w is a property characteristic of a particular material; it is related to the threshold frequency through $w = h\nu_0$.

The theory of light quanta also serves to explain the Compton effect; this experiment demonstrated that a light quantum, or a photon, behaves like a particle, in the same sense as an electron or a proton is a particle. Compton arranged for X-rays of defined wavelength λ to fall on a graphite target; he discovered that scattered X-rays have a longer wavelength λ' that depends on the scattering angle θ.

We present Figure 13.1 to explain the Compton effect. The relation between energy and momentum according to special relativity is

$$E^2 = (mc^2)^2 + (pc)^2. \tag{13.16}$$

According to the light-quantum theory, an X-ray is a photon moving at the speed of light, and its rest mass must equal zero. Each photon carries energy $E = h\nu$; the momentum of a photon is thus

$$p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda}. \tag{13.17}$$

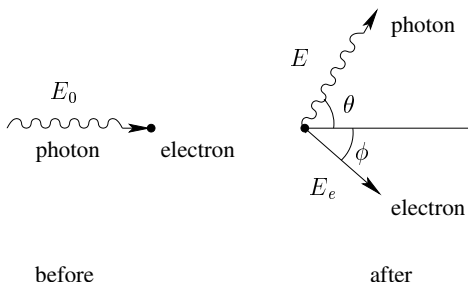


Figure 13.1: Compton effect.

Scattering occurs when a photon collides with an electron of mass m. From relativistic kinematics in Section 12.2, both relativistic energy and momentum are conserved. Let the energy of the incident X-ray be E_0, energy of the scattered X-ray E and energy of the scattered electron E_e; conservation of energy yields

$$E_0 + mc^2 = E + E_e. \tag{13.18}$$

With an incident photon directed along the x axis, conservation of momentum in the x component produces

$$\frac{E_0}{c} = p_e \cos\phi + \frac{E}{c}\cos\theta, \tag{13.19}$$

and for the y component,

$$p_e \sin\phi = \frac{E}{c}\sin\theta; \tag{13.20}$$

with p_e we denote the momentum that an electron acquires after the collision, which is related to E_e through

$$E_e^2 = (mc^2)^2 + p_e^2 c^2. \tag{13.21}$$

Solving equations (13.18), (13.19) and (13.20) simultaneously, which involves extensive calculation, we obtain

$$\lambda = \lambda_0 + \frac{h}{mc}(1 - \cos\theta). \tag{13.22}$$

We define the quantity

$$\lambda_{\mathrm{C}} \equiv \frac{h}{mc} = 2.43 \times 10^{-12}\ \mathrm{m}, \tag{13.23}$$

as the Compton wavelength.

Worksheet 13.2 Before defining equations (13.18), (13.19) and (13.20), we define E_e, E and E_0 in terms of p_e, λ and λ_0. We have three equations, but four unknowns λ, p_e, θ and ϕ. Seeking a relation between λ and θ, we employ the `solve` command in the form of `Soln1`.

```
> Ene := sqrt((m*c^2)^2 + (pe*c)^2);
```

$$Ene := \sqrt{m^2\,c^4 + pe^2\,c^2}$$

```
> En := h*c/lambda; En0 := h*c/lambda0;
```

$$En := \frac{h\,c}{\lambda}$$

$$En0 := \frac{h\,c}{\lambda 0}$$

```
> Eq1 := En0 + m*c^2 = En + Ene;
```

$$Eq1 := \frac{h\,c}{\lambda 0} + m\,c^2 = \frac{h\,c}{\lambda} + \sqrt{m^2\,c^4 + pe^2\,c^2}$$

```
> Eq2 := pe*sin(phi) = En/c*sin(theta);
```

$$Eq2 := pe\sin(\phi) = \frac{h\sin(\theta)}{\lambda}$$

```
> Eq3 := En0/c = pe*cos(phi) + En/c*cos(theta);
```

$$Eq3 := \frac{h}{\lambda 0} = pe\cos(\phi) + \frac{h\cos(\theta)}{\lambda}$$

```
> Soln1 := solve({Eq1, Eq2, Eq3}, {lambda, phi, pe}):
> assign(Soln1);
> collect(lambda, {h, m, c});
```

$$\lambda 0 + \frac{(-\cos(\theta) + 1)\,h}{c\,m}$$

13.3 Wave–Particle Duality

Maxwell's equations provide strong theoretical evidence that light is an electromagnetic wave, because electric and magnetic fields, in a region free of sources, conform to a wave equation with the speed of light c. This theory clearly explains phenomena of physical optics such as interference and diffraction, but classical electromagnetism failed to explain blackbody radiation, the photoelectric effect and the Compton effect: for this one requires Einstein's particle theory of light. To define a particle, we specify its momentum p, which is related to wavelength of the light by

$$p = \frac{h}{\lambda}. \tag{13.24}$$

In 1923, de Broglie proposed an association of a wave with each moving particle, corresponding to Einstein's association of particle characteristics of a light wave. A particle with momentum p has an associated wave, called a matter wave, with wavelength

$$\lambda = \frac{h}{p}. \tag{13.25}$$

Although one might find various representations of this formula, one should recognize that this relation is a fundamental postulate that cannot be derived.

This postulate of a matter wave soon elicited experimental support, first by Davisson and Germer in the diffraction of electrons. They discovered that electrons of energy E scattered from crystalline nickel exhibited a diffraction pattern similar to that of X-ray scattering. From that pattern they calculated the wavelength to be

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{p}. \tag{13.26}$$

The result was verified independently by G. P. Thompson, using electrons transmitted through metallic films.

Evidence for the wave nature of light had long been abundant, but the discovery of the Compton effect gives indisputable evidence that light manifests a particle property in certain experiments. While electrons were supposed to be particles, their wave aspects were incontrovertible from experiments on diffraction of electrons, and likewise for more massive neutrons from neutron diffraction experiments. Although baffling, this wave–particle duality is a universal property of all particles, which has been consistently verified experimentally. The wave–particle duality motivates a philosophical interpretation of quantum mechanics, most famously the complementarity principle of Bohr and his Copenhagen School. We refrain from exploring this topic, to which is devoted abundant literature, but we must understand the connection between a particle, specified by its energy E and momentum p, and a wave, specified by its frequency ν and wavelength λ, in accordance with the Einstein–de Broglie relation,

$$E \longleftrightarrow h\nu, \quad p \longleftrightarrow \frac{h}{\lambda}, \tag{13.27}$$

or

$$E \longleftrightarrow \hbar\omega, \quad p \longleftrightarrow \hbar k. \tag{13.28}$$

Recall the uncertainty principle for a wave in Section 10.3.3, which is purely a property of the Fourier integral, to be

$$\Delta x\, \Delta k \geq \frac{1}{2}, \quad \Delta t\, \Delta\omega \geq \frac{1}{2}. \tag{13.29}$$

Using the Einstein–de Broglie relation, we directly obtain this result,

$$\boxed{\Delta x\, \Delta p \geq \frac{\hbar}{2}, \quad \Delta t\, \Delta E \geq \frac{\hbar}{2}}, \tag{13.30}$$

known as Heisenberg's principle of uncertainty. This principle is the foundation of quantum mechanics; as it is related to an intrinsic property of any wave, the origin of quantum uncertainty is rooted in wave–particle duality.

13.4 Bohr Model of the Hydrogen Atom

In 1853, Ångström studied emission spectra of hydrogen in a glass tube excited by electric sparks, and observed four lines, one in the red, one in the blue-green and two in the violet. In 1885, J. J. Balmer fitted wavelengths of these four lines with a simple formula,

$$\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right), \tag{13.31}$$

where n takes values 3, 4, 5, 6 for the four lines; the value of this Rydberg constant R is $10\,967\,757.6\,\mathrm{m}^{-1}$.

Long before the discovery of the atomic nucleus, a planetary model for atoms had been proposed: an atom was supposed to be analogous to the solar system. About 1911, Rutherford conducted experiments using α-particles to bombard thin foils of various substances; his results indicated that all the positive charge of an atom and essentially all its mass are concentrated in a small region in the center called an atomic nucleus. A massive nucleus and a light, orbiting electron therefore serves as a model for a hydrogen atom. According to this model, the Coulomb force provides centripetal acceleration v^2/r for circular motion,

$$\frac{1}{4\pi\epsilon_0}\frac{e^2}{r^2} = m\frac{v^2}{r}; \tag{13.32}$$

the total energy is the sum of the kinetic energy and the potential energy,

$$E = \frac{1}{2}mv^2 - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}. \tag{13.33}$$

This planetary model for the hydrogen atom has a serious flaw. According to classical electromagnetic theory, an accelerating electron emits radiation. From equation (10.75), an electric charge e undergoing oscillation with angular frequency ω and amplitude x_0 along a line radiates energy at a rate

$$-\frac{dE}{dt} = \frac{\mu_0 e^2 x_0^2 \omega^4}{12\pi c}. \tag{13.34}$$

Because energy radiated must be at the expense of mechanical energy of the electron, the electron would spiral into the nucleus: the planetary model for an atom is unstable.

In 1913 Bohr achieved an interpretation of the spectrum of atomic hydrogen by proposing the existence of *stationary states*, which correspond to orbits in which the electron does not radiate energy. For such an orbit, the angular momentum satisfies this condition:

$$L = mvr = \frac{nh}{2\pi}, \tag{13.35}$$

where the quantum number n is an integer.

With Bohr's additionally imposed requirement, we solve equations (13.32), (13.33) and (13.35) simultaneously, to obtain

$$r_n = n^2 \frac{h^2 \epsilon_0}{\pi m e^2}, \tag{13.36}$$

$$v_n = \frac{1}{n} \frac{e^2}{2h\epsilon_0}, \tag{13.37}$$

$$E_n = -\frac{1}{n^2} \frac{me^4}{8\epsilon_0^2 h^2}. \tag{13.38}$$

Taking r_1 to denote the radius of an orbit for which $n = 1$, we define this value

$$a_0 \equiv r_1 = \frac{h^2 \epsilon_0}{\pi m e^2} = 0.5291772083 \times 10^{-10} \text{ m}, \tag{13.39}$$

as the Bohr radius, and $-E_1$, being the negative of energy for the same state with $n = 1$, which is

$$-E_1 = \frac{me^4}{8\epsilon_0^2 h^2} = 2.179871902 \times 10^{-18} \text{ J}, \tag{13.40}$$

as the Rydberg energy; this energy in terms of electron volt is 13.60569172 eV.

Worksheet 13.3 With Maple we readily solve three equations for three unknowns – r, v and E.

```
> Eq1 := m*v*r = n*h/(2*Pi);
```

$$Eq1 := m\,v\,r = \frac{n\,h}{2\,\pi}$$

```
> Eq2 := e^2/(4*Pi*epsilon[0]*r^2) = m*v^2/r;
```

$$Eq2 := \frac{1}{4}\,\frac{e^2}{\pi\,\varepsilon_0\,r^2} = \frac{m\,v^2}{r}$$

```
> Eq3 := En = 1/2*m*v^2 - e^2/(4*Pi*epsilon[0]*r);
```

$$Eq3 := En = \frac{m\,v^2}{2} - \frac{1}{4}\,\frac{e^2}{\pi\,\varepsilon_0\,r}$$

```
> Soln1 := solve({Eq1, Eq2, Eq3}, {r, v, En});
```

$$Soln1 := \left\{ r = \frac{n^2\,h^2\,\varepsilon_0}{e^2\,m\,\pi},\ En = -\frac{1}{8}\,\frac{e^4\,m}{\varepsilon_0{}^2\,n^2\,h^2},\ v = \frac{1}{2}\,\frac{e^2}{n\,h\,\varepsilon_0} \right\}$$

For the reader to evaluate the above quantities numerically, the relevant physical constants are listed in Appendix A. This problem represents a conjunction of Newtonian mechanics, classical electromagnetism and quantum theory. If one ensures that all input is in SI units, the results will also have the appropriate SI units.

The energy E_n of a stationary state is characterized by a quantum number n. According to Bohr's model, a spectral line corresponds to a transition between two stationary states, such that the difference between two distinct energies becomes the energy of a photon,

$$\Delta E = \frac{me^4}{8\epsilon_0^2 h^2}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) = h\nu. \tag{13.41}$$

Dividing this equation by hc, we obtain

$$\frac{\Delta E}{hc} = \frac{1}{\lambda} = \frac{me^4}{8\epsilon_0^2 h^3 c}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right), \tag{13.42}$$

which is equivalent to the formula of Balmer. The Rydberg constant is identified as

$$R_\infty = \frac{me^4}{8\epsilon_0^2 h^3 c}, \tag{13.43}$$

and its numerical value is $R_\infty = 10\,973\,731.6\ \mathrm{m}^{-1}$. Although this value is near the value from experiments cited in the beginning of this section, there is a small discrepancy. The subscript ∞ in the Rydberg constant R above, pertains to an atomic nucleus of infinite mass. Although a nucleus is massive relative to an electron (the mass of a proton is 1836 times that of an electron), it is not fixed in space. As discussed in Section 4.3, a two-body problem can be equivalently treated as that of one body fixed in space and another moving with the reduced mass. The reduced mass μ for a system consisting of m and M is

$$\mu = \frac{mM}{m+M}. \tag{13.44}$$

The Rydberg constant therefore should be modified to

$$R_M = \frac{\mu}{m}R_\infty = \frac{R_\infty}{1+\dfrac{m}{M}}. \tag{13.45}$$

We leave it as an exercise for the reader to evaluate the Rydberg constant for the hydrogen atom. H. C. Urey discovered heavy hydrogen, or deuterium, in 1931: he observed spectral lines slightly displaced from those of ordinary hydrogen. From the Rydberg constant, he deduced the existence of a chemical element identical to hydrogen but with atoms in which the nucleus has twice the mass.

Although Bohr's theory gives the correct energy levels of the hydrogen atom, one-electron ions such as He^+ and Li^{++}, and even artificially produced muonic atoms, it provides no satisfactory method for calculating the intensity of the corresponding spectral line. Moreover, attempts to apply it to the helium atom produced results which deviated greatly from experiment, and from observation of rotational spectra of diatomic molecules, the rotational energy levels are not proportional to J^2 ($J = 0, 1, 2, \ldots$) as required by Bohr's postulate about the quantization of angular momentum. Instead they are proportional to $J(J+1)$. By 1923, it was recognized that Bohr's theory needed to be improved and extended. The search for a better theory was soon successful, with the discovery of quantum mechanics, which is the subject of the subsequent chapters.

13.5 Dielectrics and Paramagnetism

To apply Maxwell's equations to a medium, we introduce the polarization $\mathbf{P}$ and the magnetization $\mathbf{M}$. The magnetization $\mathbf{M}$ is defined as the net magnetic dipole moment per unit volume, and the polarization $\mathbf{P}$ is the net electric dipole moment per unit volume. Each of $\mathbf{M}$ and $\mathbf{P}$ is a large-scale manifestation of the dipole moments of atoms or molecules of which the material is composed. Paramagnetism typically refers to the effect that a sample develops magnetization in the direction of an externally applied field.

Although Bohr's atomic model is naive, its idea provides us with a picture of an atom as a magnetic dipole: an electron moving around a nucleus in a circular orbit constitutes a current loop (see Section 8.2). This same atomic model gives no electric dipole moment, because its average over time is zero. Some molecules, such as those of water H_2O and hydrogen chloride HCl, have a permanent electric dipole moment relative to axes fixed in the molecule. We assume that the molecule which we will discuss has a magnetic or electric dipole moment, $\mathbf{m}$ or $\mathbf{p}$ respectively. In principle, the molecular magnetic or electric dipole moment is calculable using quantum electrodynamics, but we simply adopt a value without further questioning its origin.

We can determine macroscopic quantities from averaging microscopic ones; such a technique is statistical mechanics, which is the subject of Chapter 17. For n atoms per unit volume each of which has an average moment $\langle \mathbf{m} \rangle$, then

$$\mathbf{M} = n\langle \mathbf{m} \rangle. \tag{13.46}$$

An identical treatment applies to polarization, with replacements $\mathbf{M} \to \mathbf{P}$ and $\mathbf{m} \to \mathbf{p}$. In the absence of an external field, the vector sum of dipole moments is zero because of random thermal motion. If we apply a magnetic field $\mathbf{B}$, more dipoles tend to align with the field so there is a net moment along the direction of the field. Quantitatively, the potential energy of a magnetic dipole in a field is

$$\varepsilon = -\mathbf{m} \cdot \mathbf{B} = -mB\cos\theta, \tag{13.47}$$

where θ is the angle between a dipole and the field. The probability of having a dipole in this orientation, according to the Maxwell–Boltzmann distribution, is

$$P_\varepsilon \propto \exp\left(-\frac{\varepsilon}{kT}\right) = \exp\left(\frac{mB\cos\theta}{kT}\right). \tag{13.48}$$

We define a dimensionless parameter ξ,

$$\xi \equiv \frac{mB}{kT}; \tag{13.49}$$

the average value of $\mathbf{m}$ along the direction of magnetic field, defined as the z direction, is

$$\langle m\cos\theta \rangle = \frac{\int_0^\pi m\cos\theta e^{\xi\cos\theta}\sin\theta\, d\theta}{\int_0^\pi e^{\xi\cos\theta}\sin\theta\, d\theta} = m\left(\coth\xi - \frac{1}{\xi}\right). \tag{13.50}$$

The content between the parentheses is called the Langevin function, $L(\xi)$. At the limit of high temperature and weak field, $\xi \ll 1$, it becomes

$$L(\xi) \cong \frac{1}{3}\xi + \ldots, \tag{13.51}$$

and thus

$$M_z = n\langle m\cos\theta\rangle = \frac{nm^2}{3kT}B. \tag{13.52}$$

Under such conditions the magnetization is linearly proportional to the magnetic field. The ratio of M_z to magnetic field is the magnetic susceptibility,[3] which is a dimensionless quantity. In SI units,

$$\chi_m \equiv \frac{\mu_0 M}{B} = \frac{\mu_0 n m^2}{3kT}. \tag{13.53}$$

The magnetic susceptibility χ_m is hence proportional to $1/T$; this dependence of magnetic susceptibility on reciprocal temperature is called Curie's law. Langevin's theory describes classical paramagnetism; we will make a quantum correction shortly.

Worksheet 13.4 We evaluate this integral with Maple; we observe that $\sinh^2\xi = -1 + \cosh^2\xi$ and express the result as the Langevin function. We plot this function in the next worksheet.

```
> Epr1 := exp(xi*cos(theta))*sin(theta);
```

$$Epr1 := e^{(\xi\cos(\theta))}\sin(\theta)$$

```
> Epr2 := int(Epr1*cos(theta), theta=0..Pi)/int(Epr1, theta=0..Pi);
```

$$Epr2 := \frac{\xi + 1 + (e^{\xi})^2\,\xi - (e^{\xi})^2}{\xi\,(-1 + (e^{\xi})^2)}$$

```
> Epr3 := convert(Epr2, trig):
> Epr4 := simplify(Epr3);
```

$$Epr4 := -\frac{-1 + \cosh(\xi)^2 - \xi\cosh(\xi)\sinh(\xi)}{\xi\,(-1 + \cosh(\xi)^2)}$$

```
> Epr5 := taylor(Epr4, xi);
```

$$Epr5 := \frac{1}{3}\xi + \mathrm{O}(\xi^3)$$

When an actual polar molecule is placed in an electric field, a dipole moment is induced in addition to the existing permanent dipole moment p_0; we define the atomic polarizability α to account for the induced dipole moment p_a:

$$p_a = \alpha E_{\text{local}}, \quad P_a = n\alpha E_{\text{local}}. \tag{13.54}$$

[3] The definition of magnetic susceptibility χ_m is not universally agreed; here we adopt that in *Introduction to Solid State Physics*, 7th ed., by C. Kittel, New York: Wiley, 1996, p. 417. See also a discussion in *Electricity and Magnetism*, 2nd ed., by E. M. Purcell, New York: McGraw-Hill, 1985, p. 422 and 435.

Translating the formula for magnetic susceptibility in equation (13.52) to electricity, and including the atomic polarizability, the electric susceptibility χ_e, which is dimensionless, becomes

$$\chi_e \equiv \frac{P}{\epsilon_0 E} = \frac{n\alpha}{\epsilon_0} + \frac{np_0^2}{3\epsilon_0 kT}. \tag{13.55}$$

One typically measures the relative permittivity, also known as the dielectric constant, which is defined in SI units as

$$\epsilon_r \equiv \frac{\epsilon_0 E + P}{\epsilon_0 E} = 1 + \chi_e. \tag{13.56}$$

In a gaseous state, it is satisfactory to use the macroscopic field E as the local field E_{local}, as we did in equation (13.55). In a condensed state, determination of the local field E_{local} is complicated because it is a combination of the external field and fields produced by neighboring molecules. According to a simplified model, the Debye equation for the dielectric constant is

$$3\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{n}{\epsilon_0}\left(\alpha + \frac{p_0^2}{3kT}\right), \tag{13.57}$$

see Appendix B.3 and references, for details.[4] This equation works reasonably well for some liquids, but has limited power (for instance, it fails for water) because it is based on a simplified situation. When ϵ_r is near unity, the Debye equation is approximately equivalent to equation (13.55). The right-hand side combines a contribution from induced dipole moments with a contribution from permanent dipole moments that is identical to Langevin's treatment; only the latter depends on temperature ($1/T$), and it is typically much greater than the former. Experimentally, one might determine the magnitude of the molecular dipole moment p_0 from measurement of the dielectric constant at various temperatures.

Bohr's model provides a classical analogy for understanding that the magnetic dipole moment $\mathbf{m}$ is proportional to the angular momentum of an atom, expressed as $\mathbf{J}\hbar$:

$$\mathbf{m} = g\mu_B \mathbf{J}, \tag{13.58}$$

where g is Landé's g-factor and μ_B is the Bohr magneton listed in Appendix A. One might find a "derivation" of equation (13.58) using Bohr's model, but a consistent theory for it requires quantum electrodynamics which was developed in 1948. This format allows us to include both orbital and spin angular momentum of an electron; here we use it merely as a notation.

In 1922 Stern and Gerlach performed an experiment to measure the magnetic dipole moment of individual silver atoms. They produced a beam of silver atoms and directed it through an inhomogeneous magnetic field in the z direction. According to equation (8.37), an atom experiences a force

$$F_z = \frac{\partial}{\partial z}(\mathbf{m} \cdot \mathbf{B}) = m\cos\theta \frac{\partial B}{\partial z}. \tag{13.59}$$

[4] See the Clausius–Mossotti relation, which is a special case of the Debye equation when $p_0 = 0$, in Kittel, ibid., p. 390, and a derivation in L. Pauling, *General Chemistry*, New York: Dover Publications, 1988, p. 924ff.

Classically, θ takes continuous values from 0 to π; one thus expects a smear of silver along a vertical line in the collector, and the height of the line would be proportional to m. The experimental result refutes that classical picture: only two distinct spots appeared. This phenomenon vindicates quantization of space, or quantization of angular momentum for which we will offer a theoretical explanation in Section 16.3. The essence of the Stern–Gerlach experiment is that J only takes integer (0, 1, 2, ...), or half integer ($\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, ...) values, and the component J_z along the direction of the applied field takes no value except

$$J_z = -J, -J+1, \ldots, J-1, J. \tag{13.60}$$

We write the magnetic dipole moment as

$$m \equiv g\mu_B J, \quad m_z = g\mu_B J_z. \tag{13.61}$$

Be aware of our definition of m, for which $m \neq \sqrt{\mathbf{m}\cdot\mathbf{m}}$ for a reason to be explained in Section 16.3.

Because $\cos\theta$ can assume no arbitrary value, to treat paramagnetism quantum mechanically, we replace $\cos\theta$ with $\frac{J_z}{J}$,

$$\varepsilon = -\mathbf{m}\cdot\mathbf{B} = -(g\mu_B J)B\frac{J_z}{J}, \tag{13.62}$$

for which J_z takes discrete values, and perform a summation instead of an integration:

$$\overline{m}_z = \frac{1}{Z}\sum_{J_z=-J}^{J} m\frac{J_z}{J}e^{J_z\xi/J}, \quad Z \equiv \sum_{J_z=-J}^{J} e^{J_z\xi/J}, \tag{13.63}$$

where Z is the partition function, which will be further discussed in Chapter 17. We can alternatively evaluate $\overline{m}_z$ in the above equation, on differentiation:

$$\overline{m}_z = m\frac{\partial}{\partial\xi}\ln Z = m\left[\left(1+\frac{1}{2J}\right)\coth\left\{\left(1+\frac{1}{2J}\right)\xi\right\} - \frac{1}{2J}\coth\left\{\frac{1}{2J}\xi\right\}\right]. \tag{13.64}$$

The expression between the brackets is called the Brillouin function. For high temperature or a weak field ($\xi \ll 1$), the function can be expanded as

$$\left(1+\frac{1}{2J}\right)\coth\left\{\left(1+\frac{1}{2J}\right)\xi\right\} - \frac{1}{2J}\coth\left\{\frac{1}{2J}\xi\right\} \cong \frac{1}{3}\frac{J+1}{J} + \ldots; \tag{13.65}$$

thus we regain a linear dependence of magnetization M_z on the magnetic field B,

$$M_z = n\overline{m}_z = n\frac{(gJ\mu_B)^2 B}{kT}\left(\frac{J+1}{3J}\right) = \frac{ng^2\mu_B^2 J(J+1)}{3kT}B, \tag{13.66}$$

and a dependence of the magnetic susceptibility on T^{-1} – Curie's law. This quantum result differs from that of Langevin by a factor of $\frac{J+1}{J}$. Evidently, when J approaches infinity, i.e., when $\cos\theta$ becomes continuous, we resume the classical result.

Worksheet 13.5 We evaluate the sum and derivative in equations (13.63) and (13.64); the result obtained with Maple is equivalent to the Brillouin function, but less compact than that written above. We plot the Brillouin function for various J, including the limit $J = \infty$ (dashed line), which is the Langevin function.

```
> Z := sum(exp(Jz*xi/J), Jz=-J..J);
```

$$Z := \frac{e^{(\frac{(J+1)\,\xi}{J})}}{e^{(\frac{\xi}{J})}-1} - \frac{e^{(-\xi)}}{e^{(\frac{\xi}{J})}-1}$$

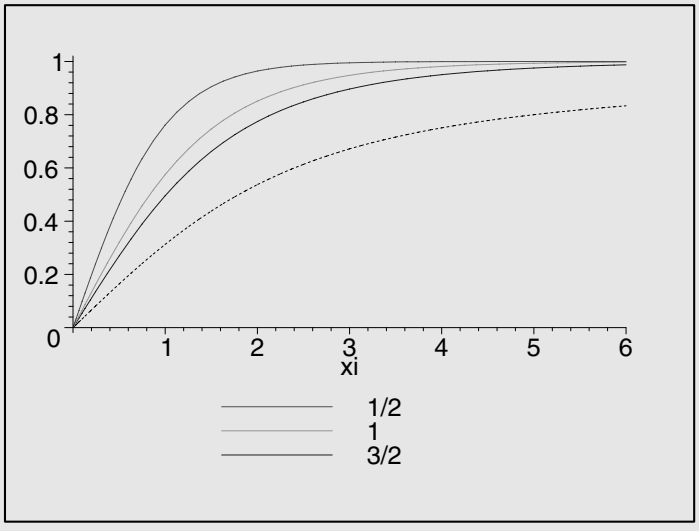
```
> Z := simplify(convert(Z, trig));
```

$$Z := \frac{\cosh\left(\frac{(J+1)\,\xi}{J}\right) + \sinh\left(\frac{(J+1)\,\xi}{J}\right) - \cosh(\xi) + \sinh(\xi)}{\cosh\left(\frac{\xi}{J}\right) + \sinh\left(\frac{\xi}{J}\right) - 1}$$

```
> Epr1 := diff(ln(Z), xi):
> Epr2 := taylor(Epr1, xi):
> simplify(Epr2);
```

$$\frac{J+1}{3\,J}\,\xi - \frac{2\,J^3+4\,J^2+3\,J+1}{90\,J^3}\,\xi^3 + \mathrm{O}(\xi^4)$$

```
> B := unapply(Epr1, J):
> plot([seq(B(J/2), J=1..3), limit(B(J), J=infinity)], xi=0..6,
> legend=["1/2","1","3/2", "infinity"]);
```



If B is large, the Brillouin function approaches 1, and M_z approaches the limiting value nm, which implies saturation of magnetization.

Exercises

1. Planck's radiation formula, equation (13.6), reproduces Wien's formula at high frequencies, and the Rayleigh–Jeans law at low frequencies.

   (a) Verify that under the condition $h\nu/kT \gg 1$,

   $$R_T(\nu)d\nu = \frac{2\pi h}{c^2}\nu^3 e^{-h\nu/kT}\,d\nu. \tag{13.67}$$

   This is Wien's radiation formula.

   (b) Verify that, under the condition $h\nu/kT \ll 1$,

   $$R_T(\nu)d\nu = \frac{2\pi\nu^2}{c^2}kT\,d\nu. \tag{13.68}$$

   This is the Rayleigh–Jeans law.

2. (a) Show that the energy density can alternatively be expressed in terms of wavelength λ, instead of frequency ν, by this formula:

   $$\rho_T(\lambda)d\lambda = \frac{8\pi hc}{\lambda^5}\frac{1}{e^{hc/\lambda kT}-1}\,d\lambda. \tag{13.69}$$

   (b) Wien's displacement law in terms of the wavelength is

   $$\lambda_{\text{max}}T = \text{constant}. \tag{13.70}$$

   Express that constant in terms of h, c, k and a numerical factor.
   Answer: $0.2014\ hc/k$.

   (c) Calculate the fraction of energy in a cavity contained within wavelengths zero and λ_{max}, according to this integral:

   $$\frac{\int_0^{\lambda_{\text{max}}}\rho_T(\lambda)\,d\lambda}{\int_0^{\infty}\rho_T(\lambda)\,d\lambda}. \tag{13.71}$$

   Answer: 0.25.

3. This exercise demonstrates another application of the use of the Lambert W function. Projectile motion with air resistance is governed by the equations

   $$\frac{d^2x}{dt^2} = -b\frac{dx}{dt}, \tag{13.72a}$$

   $$\frac{d^2y}{dt^2} = -b\frac{dy}{dt} - g. \tag{13.72b}$$

Here we assume that the air resistance is proportional to the velocity and b is the drag coefficient.[5] With initial launching velocity $v_{0x} = v_0 \cos\theta$ and $v_{0y} = v_0 \sin\theta$, solve for $x(t)$ and $y(t)$, then eliminate t to verify that the trajectory is

$$y = \frac{x}{v_{0x}}\left(v_{0y} + \frac{g}{b}\right) + \frac{g}{b^2}\ln\left(1 - \frac{bx}{v_{0x}}\right), \tag{13.73}$$

and the range R, defined as the x coordinate when $y = 0$, is

$$R = \frac{v_{0x}}{b}\left[1 + \frac{W(z)}{1 + bv_{0y}/g}\right], \tag{13.74}$$

where $W(z)$ is the Lambert function and

$$z = -\left[1 + \frac{bv_{0y}}{g}\right]\exp\left[-(1 + bv_{0y}/g)\right].$$

4. Radio astronomers have observed spectral lines of the hydrogen atom undergoing transitions between very high excited states. Calculate the wavelength and frequency of a transition between $n = 246$ and $n = 245$.

5. In the original paper on the hydrogen atom published in *Philosophical Magazine* in 1913, Bohr wrote

$$f = \frac{\sqrt{2}}{\pi}\frac{W^{3/2}}{e^2\sqrt{m}}, \tag{13.75a}$$

$$2r = \frac{e^2}{W}, \tag{13.75b}$$

where f is the frequency of revolution and W is the kinetic energy (we change the notation but retain the Gaussian system of units). Bohr imposed a quantum condition for the kinetic energy:[6]

$$W = \frac{n}{2}hf. \tag{13.76}$$

From these three equations, solve for W, f and r. The total energy E is the negative value of the kinetic energy W, thus we obtain the same energy levels and radii as in Section 13.4.

6. Evaluate the Rydberg constant R_∞, and R_M for both hydrogen and deuterium. In terms of the unified atomic mass unit (u), the rest masses for an electron, a proton, and a deuteron are 5.485803×10^{-4} u, 1.00727647 u, and 2.01355321 u, respectively.
Hint: one might employ the `ScientificConstants` package (Maple 8 or higher) for these calculations.

[5] See R. D. H. Warburton and J. Wang, "Analysis of asymptotic projectile motion with air resistance using the Lambert W function," *American Journal of Physics*, **72**, 1404–1407 (2004).

[6] Because the kinetic energy W is $\frac{1}{2}mv^2$, and for circular orbits the frequency f is $\frac{v}{2\pi r}$, simple algebraic arrangement shows that Bohr's assumption is equivalent to equation (13.35), that is $mvr = \frac{nh}{2\pi}$.

7. (a) Calculate numerical values of E_1, r_1 and v_1 for the hydrogen atom; the subscript 1 denotes the ground state.

   (b) Find the ratio of v_1 to the speed of light c; this ratio is called the fine-structure constant α.

   (c) Imagine that quantum theory suddenly fails, and an electron begins to emit radiation while orbiting a nucleus. Estimate the lifetime of such an atom from

   $$\tau \sim \frac{E_1}{2\frac{dE}{dt}}. \tag{13.77}$$

   The power of radiation dE/dt appears in equation (13.34); use r_1 for x_0, and v_1/r_1 for ω.

8. When the energy of a photon is comparable with the rest energy of an electron, quantum-mechanical modifications are necessary in photon-electron scattering. In additional to the Compton effect discussed in Section 13.2, an electron must be treated as a point particle of spin $\frac{1}{2}$ described by the Dirac equation.[7]

   (a) Verify that equation (13.22) can be written as

   $$\frac{k}{k_0} = \frac{1}{1 + x(1 - \cos\theta)}, \tag{13.78}$$

   where

   $$x \equiv \frac{hk_0}{mc} = \frac{h\nu_0}{mc^2} \tag{13.79}$$

   is the ratio of the energy of an incident photon to the rest energy of an electron.

   (b) The differential cross-section for unpolarized radiation is given by the Klein–Nishina formula for the Compton scattering:

   $$\frac{d\sigma}{d\Omega} = \frac{r_e^2}{2}\frac{k^2}{k_0^2}\left(\frac{k}{k_0} + \frac{k_0}{k} - \sin^2\theta\right), \tag{13.80}$$

   where

   $$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2}$$

   is the classical radius of the electron. The derivation of this formula is beyond the scope of this book; we simply quote the final result. Make a plot of this differential cross-section $\frac{d\sigma}{d\Omega}$ with respect to angle θ for $x = 0$, 0.25 and 1.0, which should resemble Figure 13.2(a).

[7] Jackson 1999, p. 697; W. Heitler, *The Quantum Theory of Radiation*, New York: Dover Publications, 1984, p. 219.

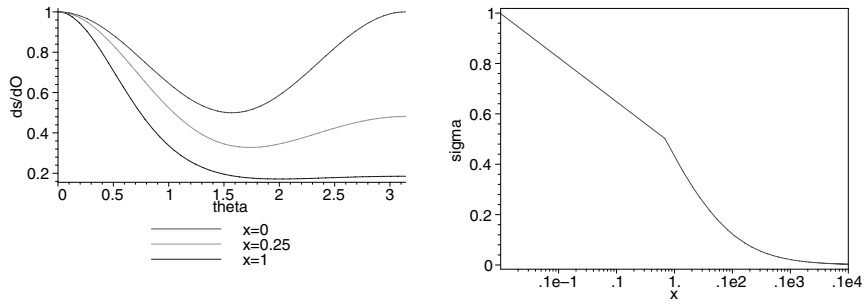


Figure 13.2: (a) Angular dependence of differential cross-section of Compton scattering. (b) Energy dependence of total cross-section of Compton scattering.

(c) The total cross-section σ is the integration of the differential cross-section over all angles:

$$\sigma = \int \frac{d\sigma}{d\Omega}\, d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \frac{d\sigma}{d\Omega} \sin\theta. \tag{13.81}$$

Verify that

$$\sigma = \sigma_T \frac{3}{4}\left\{ \frac{1+x}{x^3}\left[\frac{2x(1+x)}{1+2x} - \ln(1+2x)\right] + \frac{1}{2x}\ln(1+2x) - \frac{1+3x}{(1+2x)^2}\right\}, \tag{13.82}$$

where

$$\sigma_T = \frac{8\pi}{3} r_e^2 \tag{13.83}$$

is the Thomson cross-section. Make a plot of this total cross-section σ with respect to x, which should resemble Figure 13.2(b).

(d) Lise Meitner in 1930 made an early experimental confirmation of equation (13.82), using γ-rays of wavelength 4.7×10^{-13} m produced by ThC$''$ (^{208}Tl). Calculate x and the total cross-section σ at this energy. The success of the Klein–Nishina formula proved the necessity of negative energy solutions in the Dirac equation, which was thought to be a difficulty of the theory, before the discovery of the positron.

(e) Verify that the low-energy ($h\nu_0 \ll mc^2$) and high-energy ($h\nu_0 \gg mc^2$) limits of the total cross-section are

$$\sigma = \sigma_T \left(1 - 2x + \frac{26}{5}x^2 + \ldots\right), \quad x \ll 1, \tag{13.84}$$

and

$$\sigma = \frac{3}{8}\sigma_T \left[\frac{\ln(2x)}{x} + \frac{1}{2x}\right], \quad x \gg 1. \tag{13.85}$$

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14 Schrödinger Equation in One Dimension (I): Unbound States

In this chapter we discuss Schrödinger's formulation of quantum mechanics in one dimension. Although the matrix formulation of quantum mechanics preceded the wave formulation, the latter gained tremendous popularity immediately after its invention because of its similarity to classical waves. In our treatment, we emphasize the analogy between classical waves, introduced in earlier chapters, and quantum waves. In discussing the Gaussian wave packet according to quantum mechanics, we recall the Fourier integrals.

14.1 Formulation of Quantum Mechanics

Quantum mechanics is based on a postulate of the fundamental quantum condition; in one dimension, this fundamental quantum condition is

$$xp - px = i\hbar, \tag{14.1}$$

where x and p are operators which represent a generalized coordinate and its conjugate momentum, respectively. In Schrödinger's wave-mechanical formulation of quantum mechanics, he proposed differential operators to be associated with a generalized coordinate and its conjugate momentum. With each generalized coordinate x and generalized momentum p, we associate operators according to the following substitutions,

$$x \to x, \quad p \to \frac{\hbar}{i}\frac{\partial}{\partial x}. \tag{14.2}$$

Historically, Born and Jordan, and independently Dirac, deduced equation (14.1) from Heisenberg's formulation of quantum mechanics; according to matrix mechanics, for each physical quantity, such as x or p, there is a representative matrix.

Because, according to wave mechanics, x or p is a differential operator, such an operator requires an operand on which to operate, which we call a wave function, typically with symbol Ψ, which is in general a complex quantity. Within this wave-mechanical formulation, such a wave function completely determines the state of a physical system.

The Schrödinger equation is written as

$$H\Psi = -\frac{\hbar}{i}\frac{\partial \Psi}{\partial t}, \tag{14.3}$$

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where the Hamiltonian operator H governs the time evolution of the wave function. In classical mechanics, the Hamiltonian H for a conservative system is the sum of the kinetic energy and the potential energy,

$$H = \frac{p^2}{2m} + V(x).$$

The change of dynamical variables x and p to operators allows us to translate from a classical Hamiltonian to a quantum one, thus the Schrödinger equation becomes

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\Psi(x,t) = -\frac{\hbar}{i}\frac{\partial\Psi(x,t)}{\partial t}. \tag{14.4}$$

We emphasize that the latter development is no derivation, but an *axiom*, of nonrelativistic quantum mechanics.

The interpretation of a wave function is probabilistic. Suppose a wave function $\Psi(x,t)$ to describe a single particle; according to Born's interpretation, the probability that this particle can be found at time t in an interval between x and $x + dx$ is the complex scalar product of the wave function,

$$P(x,t)\,dx = \Psi^*(x,t)\Psi(x,t)\,dx = |\Psi(x,t)|^2\,dx, \tag{14.5}$$

where $\Psi^*(x,t)$ is the complex conjugate of $\Psi(x,t)$. We regard $|\Psi(x,t)|^2$ as the probability density. Knowledge of a wave function $\Psi(x,t)$ accordingly allows us to calculate the probability or the average of a measurement.

In many instances of physical interest, the potential energy V is not a function of time. In such a case, the Schrödinger equation can be separated into two equations; we write the general solution as a product of two functions,

$$\Psi(x,t) = \psi(x)f(t). \tag{14.6}$$

Substituting equation (14.6) into the Schrödinger equation and dividing through by $\Psi(x,t)$, we obtain

$$\frac{1}{\psi(x)}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = -\frac{1}{f(t)}\frac{\hbar}{i}\frac{d\,f(t)}{dt}. \tag{14.7}$$

Because the left-hand side of equation (14.7) involves only the spatial variable x and the right-hand side involves only the temporal variable t, the two sides must each be equal to a constant E. Then

$$\boxed{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)}, \tag{14.8}$$

and

$$-\frac{\hbar}{i}\frac{d}{dt}f(t) = Ef(t). \tag{14.9}$$

Equation (14.8) is called the time-independent Schrödinger equation; writing it using the Hamiltonian operator, we have

$$H\psi(x) = E\psi(x), \tag{14.10}$$

which has the form of an eigenvalue equation. Each $\psi(x)$ satisfying this equation thus corresponds to an eigenfunction of the Hamiltonian, with E as the eigenvalue. The eigenvalue E of the Hamiltonian is simply the total energy of a quantum-mechanical system in a particular state with a definite energy, called a *stationary state*. The temporal part, equation (14.9), has a simple solution:

$$f(t) = \exp\left(-\frac{iEt}{\hbar}\right). \tag{14.11}$$

This equation governs the time evolution of the wave function of a stationary state.

The time-independent Schrödinger equation in one dimension is a homogeneous second-order ordinary differential equation; solving for $\psi(x)$ and E in such an equation for various potential-energy functions $V(x)$, of which a formal term is an eigenvalue problem, is the topic of this and subsequent two chapters.

The wave function $\psi(x)$ must be well-behaved: it and its derivative must be finite everywhere. In addition, $\psi(x)$ must be continuous, and in general its derivative $\frac{d\psi(x)}{dx}$ must also be continuous except for some special situations (e.g., an infinite potential well discussed in Section 15.2).

14.2 Zero Potential and Plane Waves

For a zero potential $V = 0$, the Schrödinger equation is readily solved. Let the solution take the form

$$\psi(x) = \exp\left(\frac{ipx}{\hbar}\right). \tag{14.12}$$

Substituting this in equation (14.8), we verify that the proposed function is indeed an eigenfunction of H, and obtain the eigenvalue E, which yields an obvious relation

$$E = \frac{p^2}{2m}, \tag{14.13}$$

just as for translational kinetic energy in classical mechanics. The complete wave function is

$$\Psi(x,t) = \psi(x)f(t) = \exp\left[\frac{i(px - Et)}{\hbar}\right]. \tag{14.14}$$

Each such function describes a state where the particle has a definite energy E and momentum p. This function has exactly the same form as a classical plane wave; comparing this wave function with a classical plane wave in complex notation,

$$\exp[i(kx - \omega t)],$$

we find the corresponding angular frequency ω and wave vector k of this quantum wave function:

$$\omega = \frac{E}{\hbar} = \frac{p^2}{2m\hbar}, \quad k = \frac{p}{\hbar}. \tag{14.15}$$

The wavelength corresponding to this quantum wave function is h/p, which is the de Broglie wavelength of a free particle.

This solution can describe an ideal experiment, in which an accelerator situated at $x = -\infty$ produces a mono-energetic beam of electrons emitted in the positive x direction. For each such electron, its particle concept is completely irrelevant: because $P(x,t) = \Psi^*(x,t)\Psi(x,t)$ is a constant, the probability of finding this electron in an interval is the same everywhere. We can understand this wave–particle duality according to the uncertainty principle,

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{14.16}$$

Because we know the energy and momentum exactly, that is, $\Delta p = 0$, the position must be completely uncertain; that is, $\Delta x = \infty$.

14.3 Step Potential

For an experimental condition, suppose that a source of plane waves is located at $x = -\infty$, emitting waves with a specific energy E in the positive x direction. We describe a step potential with this discontinuous function,

$$V(x) = \begin{cases} V_0, & x > 0, \\ 0, & x < 0, \end{cases} \tag{14.17}$$

where the step height $V_0 > 0$. Denoting $x < 0$ as region 1 and $x > 0$ as region 2, we seek a wave function $\psi(x)$ that satisfies the Schrödinger equation in both regions 1 and 2.

14.3.1 Step Potential ($E > V_0$)

We first consider a situation in which the total energy E is greater than the potential step height V_0. In region 1, the solution of the Schrödinger equation is the same as that in the problem of zero potential discussed earlier, for which the solution is a plane wave with a wave vector

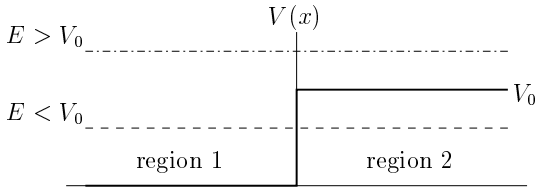


Figure 14.1: Step potential.

$k_1 = p_1/\hbar$. Replacing k_1 with $-k_1$, we obtain another class of solution. We therefore write the solution in region 1 as

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}. \tag{14.18}$$

In this solution, the first term represents a wave traveling in the positive x direction, whereas the second term represents a wave traveling in the negative x direction.

In region 2, the solution has the form

$$\psi_2(x) = Ce^{ik_2x}. \tag{14.19}$$

Because we assume that incident waves emanate from a source at $x = -\infty$, we reject the solution e^{-ik_2x}: there is only a wave traveling in the positive x direction in region 2. This solution exhibits an oscillatory behavior.

Directly substituting $\psi(x)$ into the Schrödinger equation, we obtain

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, \tag{14.20}$$

and

$$k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}. \tag{14.21}$$

Because $p = \hbar k$, we again verify an obvious relation $E = p_1^2/2m$ in free space, and more generally $E - V_0 = p_2^2/2m$. In the literature of quantum mechanics, some authors prefer to use the momentum p and others prefer to use the wave vector k to express a plane wave; they merely differ by a factor of $\hbar$.

The wave function $\psi(x)$ must be continuous. At the boundary of the barrier $x = 0$, we have

$$\psi_1(0) = \psi_2(0), \quad A + B = C. \tag{14.22}$$

The first derivative of $\psi(x)$ must also be continuous; we have

$$\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left.\frac{d\psi_2}{dx}\right|_{x=0}, \quad k_1(A - B) = k_2C. \tag{14.23}$$

We have three unknowns A, B and C, but only two equations. We can still solve equations (14.22) and (14.23) simultaneously, and obtain B and C in terms of A:

$$B = \frac{k_1 - k_2}{k_1 + k_2} A, \tag{14.24}$$

$$C = \frac{2k_1}{k_1 + k_2} A. \tag{14.25}$$

The transmission coefficient T is defined as

$$T = \frac{k_2 C^* C}{k_1 A^* A}, \tag{14.26}$$

where the asterisk indicates the complex conjugate. Thus

$$T = \frac{4k_1 k_2}{(k_1 + k_2)^2}. \tag{14.27}$$

The reflection coefficient R is defined as

$$R = \frac{B^* B}{A^* A} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}. \tag{14.28}$$

Recall that k_1 and k_2 are expressed in terms of E and V_0; we leave it as an exercise to plot R and T as a function of the ratio E/V_0.

Worksheet 14.1 To undertake the above calculations with Maple, we apply the arrow operator `->` to define a function. The differential operator `D` is useful in many worksheets in this and other chapters: with it we can impose the continuity condition for the first derivative of the function at the boundaries. There are three unknowns A, B and C, but only two equations; we find ratios so as to express B and C in terms of A. The `assign` command changes `=` to `:=`, so that we can call the results `B` and `C` directly from `Soln1`. The `conjugate` command is repeatedly used in quantum-mechanical problems.

```
> assume(k1>0, k2>0);
> psi1 := x-> A*exp(I*k1*x) + B*exp(-I*k1*x);
```

$$\psi 1 := x \to A\, e^{(k1\, x\, I)} + B\, e^{(-I\, k1\, x)}$$

```
> psi2 := x-> C*exp(I*k2*x);
```

$$\psi 2 := x \to C\, e^{(k2\, x\, I)}$$

```
> Eq1 := psi1(0) = psi2(0);
```

$$Eq1 := A + B = C$$

```
> Eq2 := D(psi1)(0)= D(psi2)(0);
```

$$Eq2 := A\, k1\, I - B\, k1\, I = C\, k2\, I$$

```
> Soln1 :=solve({Eq1, Eq2}, {B, C});
```

$$Soln1 := \left\{ B = \frac{A\,(k1 - k2)}{k1 + k2},\ C = \frac{2\,A\,k1}{k1 + k2} \right\}$$

```
> assign(Soln1);
> R := conjugate(B)*B/(conjugate(A)*A);
```

$$R := \frac{(k1 - k2)^2}{(k1 + k2)^2}$$

```
> T := k2*conjugate(C)*C/(k1*conjugate(A)*A);
```

$$T := \frac{4\,k2\,k1}{(k1 + k2)^2}$$

```
> simplify(R + T);
```

$$1$$

We verify that the sum of R and T is unity.

14.3.2 Step Potential ($E < V_0$)

If the total energy E is less than the step potential height V_0, the wave function in region 1 retains the same form. In region 2, the wave function becomes

$$\psi_2(x) = Ce^{-\kappa_2 x}. \tag{14.29}$$

This solution manifests an exponential decay. Another possible solution $e^{+\kappa_2 x}$, signifying exponential growth, must be rejected, otherwise the solution diverges at $x = \infty$. Direct substitution of this solution into the Schrödinger equation yields

$$\kappa_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \tag{14.30}$$

Applying boundary conditions at $x = 0$ again yields

$$\psi_1(0) = \psi_2(0), \quad A + B = C. \tag{14.31}$$

$$\psi_1'(0) = \psi_2'(0), \quad ik_1(A - B) = -\kappa_2 C. \tag{14.32}$$

Solving equations (14.31) and (14.32) produces

$$B = \frac{ik_1 + \kappa_2}{ik_1 - \kappa_2} A, \tag{14.33}$$

$$C = \frac{2ik_1}{ik_1 - \kappa_2} A. \tag{14.34}$$

The reflection coefficient is calculated as

$$R = \frac{B^* B}{A^* A} = 1. \tag{14.35}$$

The nonvanishing term C indicates penetration of the wave function into a classically forbidden region: there is a certain probability that the particle will be found inside the barrier.

Worksheet 14.2 Other than a minor alteration, this worksheet is the same as the preceding one.

```
> assume(k1>0, kappa2>0);
> psi1 := x-> A*exp(I*k1*x) + B*exp(-I*k1*x);
```

$$\psi 1 := x \to A\, e^{(k1\, x\, I)} + B\, e^{(-I\, k1\, x)}$$

```
> psi2 := x-> C*exp(-kappa2*x);
```

$$\psi 2 := x \to C\, e^{(-\kappa 2\, x)}$$

```
> Eq1 := psi1(0) = psi2(0);
```

$$Eq1 := A + B = C$$

```
> Eq2 := D(psi1)(0) = D(psi2)(0);
```

$$Eq2 := A\, k1\, I - B\, k1\, I = -C\, \kappa 2$$

```
> Soln1 := solve({Eq1, Eq2}, {B, C});
```

$$Soln1 := \left\{ C = \frac{-2\, I\, A\, k1}{-k1\, I + \kappa 2},\ B = -\frac{A\,(k1\, I + \kappa 2)}{-k1\, I + \kappa 2} \right\}$$

```
> assign(Soln1);
> R := conjugate(B)*B/(conjugate(A)*A);
```

$$R := 1$$

14.4 Barrier Potential

For the same source of plane waves situated at $x = -\infty$ discussed in the preceding section, we solve the Schrödinger equation for the barrier potential, which is described by this discontinuous function,

$$V(x) = \begin{cases} V_0, & 0 < x < a, \\ 0, & x < 0 \text{ or } x > a, \end{cases} \tag{14.36}$$

where V_0 is the barrier height and a is the barrier width. We denote regions with $x < 0$, $0 < x < a$ and $x > a$ as 1, 2 and 3 respectively.

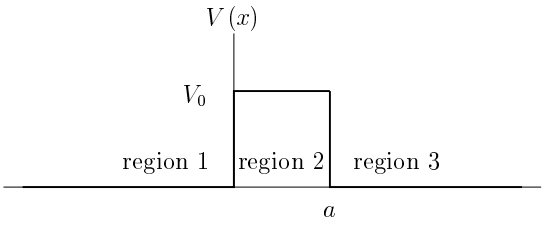


Figure 14.2: Barrier potential.

14.4.1 Barrier Potential ($E > V_0$)

The general solutions in regions 1, 2 and 3 take these forms:

$$\begin{cases} \psi_1 = Ae^{ik_1 x} + Be^{-ik_1 x}, & x < 0, \\ \psi_2 = Fe^{ik_2 x} + Ge^{-ik_2 x}, & 0 < x < a, \\ \psi_3 = Ce^{ik_1 x}, & x > a. \end{cases} \tag{14.37}$$

We can assign A to be unity without loss of generality, so that we only have four unknowns. We leave it to the reader to verify that k_1 and k_2 are identical to those in Section 14.3.1. The coefficients are again determined by the continuity conditions of ψ and ψ' at points $x = 0$ and $x = a$, namely

$$\psi_1(0) = \psi_2(0), \quad \psi_1'(0) = \psi_2'(0),$$

$$\psi_2(a) = \psi_3(a), \quad \psi_2'(a) = \psi_3'(a).$$

From these four equations, we solve for B, C, F and G (we set $A \equiv 1$). The transmission coefficient T is defined as

$$T = \frac{k_1 C^* C}{k_1 A^* A} = |C|^2. \tag{14.38}$$

We use Maple to solve these equations and to evaluate T, which is a task which is very tedious to perform manually.

Worksheet 14.3 This worksheet employs the same commands as the preceding worksheets.

```
> assume(a>0, k1>0, k2>0); additionally(k1>k2);
> psi1 := x -> exp(I*k1*x) + B*exp(-I*k1*x);
```

$$\psi 1 := x \to e^{(k1\,x\,I)} + B\,e^{(-I\,k1\,x)}$$

```
> psi2 := x -> F*exp(I*k2*x) + G*exp(-I*k2*x);
```

$$\psi 2 := x \to F\,e^{(k2\,x\,I)} + G\,e^{(-I\,k2\,x)}$$

```
> psi3 := x -> C*exp(I*k1*x);
```

$$\psi 3 := x \to C\, e^{(k1\, x\, I)}$$

```
> Soln1 :=solve({psi1(0)=psi2(0), psi2(a)=psi3(a),
> D(psi1)(0)=D(psi2)(0), D(psi2)(a)=D(psi3)(a)}, {B,C,F,G});
```

$$Soln1 := \left\{ F = -\frac{2\,(k1+k2)\,k1}{\%3},\ G = \frac{2\,k1\,(e^{(k2\,a\,I)})^2\,(k1-k2)}{\%3},\right.$$
$$\left. C = -\frac{4\,k2\,k1\,e^{(k2\,a\,I-k1\,a\,I)}}{\%3},\ B = \frac{-\%2-k1^2+\%1+k2^2}{\%3} \right\}$$
$$\%1 := k1^2\,(e^{(k2\,a\,I)})^2$$
$$\%2 := k2^2\,(e^{(k2\,a\,I)})^2$$
$$\%3 := -2\,k1\,(e^{(k2\,a\,I)})^2\,k2 + \%2 - 2\,k1\,k2 - k1^2 + \%1 - k2^2$$

```
> assign(Soln1);
> C;
```

$$-\frac{4\,k2\,k1\,e^{(k2\,a\,I-k1\,a\,I)}}{-2\,k1\,(e^{(k2\,a\,I)})^2\,k2 + k2^2\,(e^{(k2\,a\,I)})^2 - 2\,k1\,k2 - k1^2 + k1^2\,(e^{(k2\,a\,I)})^2 - k2^2}$$

```
> T := C*conjugate(C):
> T := evalc(T):
> T := simplify(T);
```

$$T := -\frac{4\,k2^2\,k1^2}{-2\,k1^2\,k2^2\cos(k2\,a)^2 + k2^4\cos(k2\,a)^2 + k1^4\cos(k2\,a)^2 - 2\,k2^2\,k1^2 - k1^4 - k2^4}$$

After manually combining $1-\cos^2(k_2a) = \sin^2(k_2a)$ in the Maple output, we obtain the expression for the transmission coefficient T:

$$T = \frac{4k_1^2k_2^2}{(k_1^2-k_2^2)^2\sin^2 ak_2 + 4k_1^2k_2^2}. \tag{14.39}$$

14.4.2 Barrier Potential ($E < V_0$)

For the $E < V_0$ case, the solution in region $0 < x < a$ is replaced by

$$\psi_2 = Fe^{\kappa_2 x} + Ge^{-\kappa_2 x}, \quad 0 < x < a. \tag{14.40}$$

Again k_1 and κ_2 are identical to those in Section 14.3.2. Applying exactly the same continuity conditions at the boundaries, we can solve for the coefficients. The coefficient T for

transmission past the barrier is

$$T = \frac{4k_1^2\kappa_2^2}{(k_1^2 - \kappa_2^2)^2 \sinh^2 a\kappa_2 + 4k_1^2\kappa_2^2}. \tag{14.41}$$

We can use Maple to obtain an identical mathematical result, although in a much less compact form as shown above. We will treat this problem numerically shortly. The fact that T is nonvanishing is an example of quantum-mechanical tunneling.

14.5 Summary of Stationary States

In all examples we have seen so far, we have piecewise-constant potentials in one dimension. Particles are described by plane waves, that is, in a state with specific energy E. To find $\psi(x)$, we first write a general solution: if $E > V_0$, the solution is oscillatory, and if $E < V_0$, the solution is exponential. To illustrate explicitly, for the problem of a rectangular barrier in Section 14.4.2, we have

$$\psi(x) = \begin{cases} \psi_1 = 1e^{ik_1 x} + Be^{-ik_1 x}, & x < 0, \\ \psi_2 = Fe^{\kappa_2 x} + Ge^{-\kappa_2 x}, & 0 < x < a, \\ \psi_3 = Ce^{ik_1 x}, & x > a. \end{cases} \tag{14.42}$$

We then evaluate coefficients B, C, F, and G on applying the continuity requirement at each boundary, and solve for them in terms of k_1 and κ_2, which are themselves expressed in terms of total energy E and potential height V_0,

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, \quad \kappa_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \tag{14.43}$$

The complete wave function is

$$\Psi(x,t) = \psi(x)f(t). \tag{14.44}$$

The function $f(t)$ produces sinusoidal oscillation of $\psi(x)$ at frequency $\omega = E/\hbar$. The probability density is

$$P(x,t) = \Psi^*(x,t)\Psi(x,t) = \psi^*(x)e^{iEt/\hbar}\psi(x)e^{-iEt/\hbar} = \psi^*(x)\psi(x). \tag{14.45}$$

For a state with definite energy, the probability density is independent of time, hence justifying the name stationary state.

Example 14.1 With this numerical example, we illustrate a solution of the Schrödinger equation. Suppose an accelerator at $x = -\infty$ produces a mono-energetic beam of electrons with energy $E = 6$ eV $= 6 \times 1.6 \times 10^{-19}$ J. Let this electron beam be incident on a potential barrier of height $V_0 = 10$ eV $= 10 \times 1.6 \times 10^{-19}$ J, and width 1.8×10^{-10} m.

Worksheet 14.4 To evaluate the coefficients, we solve a system of equations; notice that we use `h` for $\hbar$, which is 1.055×10^{-34} J s. From the wave function, we produce an animation, from which one can observe the tunneling effect. Because this state is stationary, the probability density is independent of time.

```
> m := 9.1e-31; V0 := 10*1.6e-19; h := 1.055e-34; a := 1.8e-10;
```

$$m := 0.91\,10^{-30}$$
$$V0 := 0.160\,10^{-17}$$
$$h := 0.1055\,10^{-33}$$
$$a := 0.18\,10^{-9}$$

```
> En := .6*V0; w := En/h; k1:=sqrt(2*m*En)/h;
> kappa2:=sqrt(2*m*(V0-En))/h;
```

$$En := 0.960\,10^{-18}$$
$$w := 0.9099526066\,10^{16}$$
$$k1 := 0.1252907044\,10^{11}$$
$$\kappa 2 := 0.1022994318\,10^{11}$$

```
> psi1 := x -> exp(I*k1*x) + B*exp(-I*k1*x);
```

$$\psi 1 := x \to e^{(k1\,x\,I)} + B\,e^{(-I\,k1\,x)}$$

```
> psi2 := x -> F*exp(kappa2*x) + G*exp(-kappa2*x);
```

$$\psi 2 := x \to F\,e^{(\kappa 2\,x)} + G\,e^{(-\kappa 2\,x)}$$

```
> psi3 := x -> C*exp(I*k1*x);
```

$$\psi 3 := x \to C\,e^{(k1\,x\,I)}$$

```
> Soln1 := solve({psi1(0) = psi2(0), psi2(a) = psi3(a), D(psi1)(0)
> = D(psi2)(0), D(psi2)(a)= D(psi3)(a)}, {B, C, F, G});
```

$$\begin{aligned} Soln1 := \{&G = 1.163524404 - 0.9688460132\,I,\\ &B = 0.1815481747 - 0.9352973513\,I,\\ &F = 0.01802377044 + 0.03354866193\,I,\\ &C = -0.1436753713 - 0.2676126167\,I\} \end{aligned}$$

```
> assign(Soln1);
> psi1(x);
```

$$e^{(0.1252907044\,10^{11}\,I\,x)} + (0.1815481747 - 0.9352973513\,I)\,e^{(-0.1252907044\,10^{11}\,I\,x)}$$

```
> Psi1(x,t) := psi1(x)*exp(-I*w*t);
```

$$\begin{aligned} \Psi 1(x,\,t) := \Big(&e^{(0.1252907044\,10^{11}\,I\,x)}\\ &+(0.1815481747 - 0.9352973513\,I)\,e^{(-0.1252907044\,10^{11}\,I\,x)}\Big)e^{(-0.9099526066\,10^{16}\,I\,t)} \end{aligned}$$

```
> psi2(x);
```

$$(0.01802377044 + 0.03354866193\,I)\,e^{(0.1022994318\,10^{11}\,x)} + (1.163524404 - 0.9688460132\,I)\,e^{(-0.1022994318\,10^{11}\,x)}$$

```
> Psi2(x,t) := psi2(x)*exp(-I*w*t);
```

$$\Psi 2(x,\,t) := \left((0.01802377044 + 0.03354866193\,I)\,e^{(0.1022994318\,10^{11}\,x)} + (1.163524404 - 0.9688460132\,I)\,e^{(-0.1022994318\,10^{11}\,x)}\right) e^{(-0.9099526066\,10^{16}\,I\,t)}$$

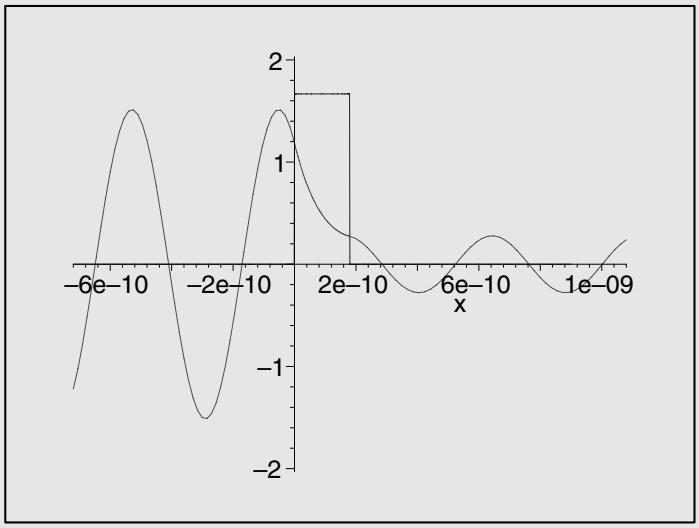
```
> psi3(x);
```

$$(-0.1436753713 - 0.2676126167\,I)\,e^{(0.1252907044\,10^{11}\,I\,x)}$$

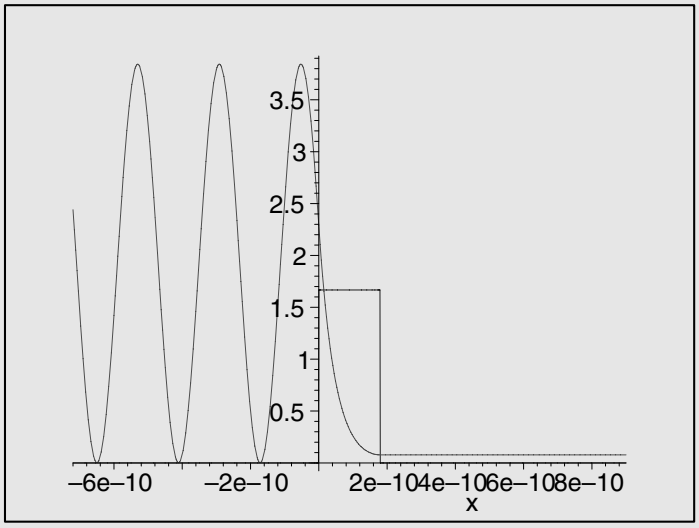
```
> Psi3(x,t) := psi3(x)*exp(-I*w*t);
```

$$\Psi 3(x,\,t) := (-0.1436753713 - 0.2676126167\,I)\,e^{(0.1252907044\,10^{11}\,I\,x)}\,e^{(-0.9099526066\,10^{16}\,I\,t)}$$

```
> br := piecewise(0<x and x<a,V0/En, x<0,0, a<x,0):
> with(plots):
Warning, the name changecoords has been redefined
> pt1 := animate(Re(Psi1(x,t)), x=-4*a..0, t=0..2*Pi/w):
> pt2 := animate(Re(Psi2(x,t)), x=0..a, t=0..2*Pi/w):
> pt3 := animate(Re(Psi3(x,t)), x=a..a+5*a, t=0..2*Pi/w):
> pbr := plot(br, x=-4*a..5*a, color=blue, thickness=2):
> display([pt1, pt2, pt3, pbr]);
```



```
> Epr11 := evalc(conjugate(Psi1(x,t))*Psi1(x,t)):
> Epr12 := simplify(Epr11):
> Epr13 := evalc(conjugate(Psi2(x,t))*Psi2(x,t)):
> Epr14 := simplify(Epr13):
> Epr15 := evalc(conjugate(Psi3(x,t))*Psi3(x,t)):
> Epr16 := simplify(Epr15):
> pb1 := plot(Epr12, x=-4*a..0):
> pb2 := plot(Epr14, x=0..a):
> pb3 := plot(Epr16, x=a..5*a):
> display([pb1, pb2, pb3, pbr]);
```



14.6 Wave Packet

The Schrödinger equation is linear: it satisfies the principle of superposition; that is, if $\Psi_1(x,t)$ is a solution of the Schrödinger equation and $\Psi_2(x,t)$ is another solution, their linear combination,

$$\Psi(x,t) = a\Psi_1(x,t) + b\Psi_2(x,t), \tag{14.46}$$

is also a solution, which represents a possible quantum state.

We have learned that in free space, for which $V = 0$, the solution of the Schrödinger equation is a plane wave:

$$\Psi(x,t) = \exp\left[\frac{i(px - Et)}{\hbar}\right]. \tag{14.47}$$

This solution is entirely unlike a particle, discussed in Section 14.2. In a similar way to a classical wave, we can form a wave packet by the superposition of plane waves. Linear combination of plane waves, which involve a Fourier integral, has been discussed extensively in Section 10.3. We here discuss the Gaussian wave packet in quantum mechanics, which is essentially identical to the treatment in classical waves. We encourage the reader to review Section 10.4 on the classical Gaussian wave packet.

The wave function of a Gaussian wave packet in coordinate space at time $t = 0$ is

$$\Psi(x,0) = f = \exp\left[-\frac{(x - x_0)^2}{2a^2} + \frac{ip_0 x}{\hbar}\right], \tag{14.48}$$

where x_0 is the mean value of the position and p_0 the mean value of the linear momentum. We can express this wave function as a superposition of plane waves. We calculate the Fourier transform $\alpha(p)$ of f as

$$\begin{aligned}\alpha(p) &= \left(\frac{1}{\sqrt{2\pi}}\right)\int_{-\infty}^{\infty} f \exp\left(\frac{-ipx}{\hbar}\right) dx \\ &= a \exp\left[-\frac{a^2}{2}\frac{(p - p_0)^2}{\hbar^2} - \frac{i(p - p_0)x_0}{\hbar}\right].\end{aligned} \tag{14.49}$$

The energy E is related to momentum p through

$$E = \frac{p^2}{2m}, \tag{14.50}$$

so the dispersion relation for the de Broglie wave is

$$\omega = \frac{E}{\hbar} = \frac{p^2}{2m\hbar}. \tag{14.51}$$

The time evolution of the Gaussian wave packet is the Fourier integral of plane waves with the Fourier transform we have just obtained. Because E depends on p as seen above, the term containing E in the plane wave must remain inside the integral. Hence,

$$\begin{aligned}\Psi(x,t) &= \left(\frac{1}{\sqrt{2\pi\hbar}}\right)\int_{-\infty}^{\infty} \alpha(p) \exp\left[\frac{-i(Et - px)}{\hbar}\right] dp \\ &= \frac{\exp\left[-\frac{(x-x_0)^2 - \frac{2ia^2 p_0 x}{\hbar} + \frac{2p_0 x_0 t}{m} + \frac{ip_0^2 a^2 t}{\hbar m}}{2a^2\left(1 + \frac{it\hbar}{ma^2}\right)}\right]}{\sqrt{1 + \frac{it\hbar}{ma^2}}}.\end{aligned} \tag{14.52}$$

From the wave function, we find the probability density $P(x,t)$ to be

$$|\Psi(x,t)|^2 = \frac{\exp\left[-\frac{\left(x-x_0-\frac{tp_0}{m}\right)^2}{a^2\left(1+\frac{t^2\hbar^2}{m^2a^4}\right)}\right]}{\sqrt{1+\frac{t^2\hbar^2}{m^2a^4}}}. \tag{14.53}$$

This state is not stationary because time explicitly appears in this probability. This result is readily understandable: the Gaussian wave packet lacks a definite energy, because it constitutes plane waves having a range of energy. From the probability density, the maximum of this Gaussian function occurs at the position

$$x - x_0 = \frac{tp_0}{m},$$

which moves at a group velocity $v = p_0/m$ (which is consistent with $v = \frac{d\omega}{dk}$ where ω is in equation (14.51)). The wave packet broadens as it moves: the width at time $t = 0$ is a, and at a subsequent time t it becomes

$$a(t) = a\left[1 + \left(\frac{t\hbar}{ma^2}\right)^2\right]^{1/2}. \tag{14.54}$$

Worksheet 14.5 These integrations are readily accomplished with Maple. To ensure that improper integrals converge, one must specify the signs of pertinent variables, using the `assume` command. In this worksheet, what appears to be the Planck constant `h` is actually the reduced Planck constant $\hbar$ in the above formulation.

```
> assume(a>0, h>0, m>0, t>0); assume(x, real, p, real, x0, real,
> p0, real):
> f := exp(I*p0*x/h-(x-x0)^2/(2*a^2));
```

$$f := e^{\left(\frac{p0\,x\,I}{h} - \frac{(x-x0)^2}{2\,a^2}\right)}$$

```
> alpha := 1/sqrt(2*Pi)*int(exp(-I*p*x/h)*f,
x=-infinity..infinity):
> alpha := simplify(alpha);
```

$$\alpha := e^{\left(\frac{-1/2\,I\,(p-p0)\,(-p\,a^2\,I+p0\,a^2\,I+2\,x0\,h)}{h^2}\right)}\,a$$

```
> En := p^2/(2*m);
```

$$En := \frac{p^2}{2\,m}$$

```
> psi := 1/(sqrt(2*Pi)*h)*int(alpha*exp(I*(p*x/h-En/h*t)),
> p=-infinity..infinity):
```

```
> psi := simplify(psi);
```

$$\psi := \frac{e^{\left(\frac{1/2\, I\, (-p0^2\, a^2\, t+2\, I\, p0\, x0\, h\, t+2\, m\, p0\, a^2\, x+m\, x0^2\, h\, I-2\, I\, m\, x0\, h\, x+m\, x^2\, h\, I)}{h\, (a^2\, m+t\, h\, I)}\right)}\, a\, \sqrt{m}}{\sqrt{a^2\, m+t\, h\, I}}$$

```
> Epr1 := psi*conjugate(psi):
> Epr2 := simplify(Epr1);
```

$$Epr2 := \frac{e^{\left(\frac{a^2\, (m\, x-m\, x0-p0\, t)^2}{(a^2\, m+t\, h\, I)\, (-a^2\, m+t\, h\, I)}\right)}\, a^2\, m}{\sqrt{a^4\, m^2+t^2\, h^2}}$$

To produce an animation, one substitutes numerical values into this result; the motion is expected to resemble the classical Gaussian wave packet in Section 10.4.

14.6.1 Reflection of Wave Packet

We consider a Gaussian wave packet moving in the positive x direction to be incident upon a step potential; we assume the average energy of this Gaussian wave packet to exceed the step potential height:

$$E_0 = \frac{p_0^2}{2m} > V_0. \tag{14.55}$$

We have discussed the problem of a plane wave entering a step potential in Section 14.3.1. For a Gaussian wave packet, the wave function results from simply summing over a range of total energy E – to be more precise, performing a Fourier integration.

For one specific energy E, the momentum in region 1 is p_1 in which $p_1^2/2m = E = p^2/2m$, and the momentum in region 2 is p_2 where $p_2^2/2m = E - V_0$. From Section 14.3.1, the complete solution in region 1 is, with A set to unity,

$$\exp\left[\frac{i(p_1 x - Et)}{\hbar}\right] + B\exp\left[\frac{i(-p_1 x - Et)}{\hbar}\right],$$

and in region 2 is

$$C\exp\left[\frac{i(p_2 x - Et)}{\hbar}\right],$$

where

$$B = \frac{p_1 - p_2}{p_1 + p_2}, \quad C = \frac{2p_1}{p_1 + p_2}; \tag{14.56}$$

see equations (14.18), (14.19), (14.24), (14.25). For a Gaussian wave packet, we have the Fourier transform $\alpha(p)$ in equation (14.49). The superposition of plane waves in regions 1

and 2 then becomes

$$\Psi_1(x,t) = \frac{1}{\sqrt{2\pi}\hbar}\int_{-\infty}^{\infty} dp\,\alpha(p)\left\{\exp\left[\frac{i(p_1x-Et)}{\hbar}\right] + \left(\frac{p_1-p_2}{p_1+p_2}\right)\exp\left[\frac{i(-p_1x-Et)}{\hbar}\right]\right\}, \quad (14.57)$$

and

$$\Psi_2(x,t) = \frac{1}{\sqrt{2\pi}\hbar}\int_{-\infty}^{\infty} dp\,\alpha(p)\left\{\left(\frac{2p_1}{p_1+p_2}\right)\exp\left[\frac{i(p_2x-Et)}{\hbar}\right]\right\}. \quad (14.58)$$

For a computational purpose, we evaluate B and C using an approximation – setting a range of momentum p at an average energy p_0; thus

$$B \cong \frac{p_0-\sqrt{p_0^2-2mV_0}}{p_0+\sqrt{p_0^2-2mV_0}}, \quad C \cong \frac{2p_0}{p_0+\sqrt{p_0^2-2mV_0}}, \quad (14.59)$$

so that they can be moved outside the integrands. Assuming the Gaussian wave packet to be sharply peaked at p_0, we perform a series expansion of p_2 in region 2,

$$p_2 = \sqrt{p^2-2mV_0} \cong \sqrt{p_0^2-2mV_0} + \left(\frac{d}{dp}\sqrt{p^2-2mV_0}\right)_{p=p_0}(p-p_0); \quad (14.60)$$

hence the integral in equation (14.58) can be evaluated exactly.

Worksheet 14.6 In this worksheet, `h` signifies $\hbar$ in the above formulation, which is anyhow set to unity. The integrals are straightforward; we use the `taylor` command to expand p_2, but retain only the linear term. We produce animations in two regions, and their combination shows the behavior of a Gaussian wave packet on encountering a barrier.

```
> assume(x, real, p, real):  assume(t>0):
> m:=1; h:=1; a:=1; x0:=-10; p0:=22; V0:=200;
```

$$m := 1$$
$$h := 1$$
$$a := 1$$
$$x0 := -10$$
$$p0 := 22$$
$$V0 := 200$$

```
> f := 1/(Pi^(1/4)*sqrt(a))*exp(I*p0*(x-x0)/h - (x-x0)^2/(2*a^2));
```

$$f := \frac{e^{(22\,I\,(x+10)-\frac{(x+10)^2}{2})}}{\pi^{(1/4)}}$$

```
> alpha := 1/sqrt(2*Pi*h)*int(exp(-I*p*x/h)*f,
> x=-infinity..infinity);
```

$$\alpha := \frac{e^{(-\frac{p^2}{2}+10\,I\,p+22\,p-242)}}{\pi^{(1/4)}}$$

```
> p2 := sqrt(p^2 - 2*m*V0);
```

$$p2 := \sqrt{p^2-400}$$

```
> p2appr := convert(taylor(p2, p=p0, 2), polynom);
```

$$p2appr := 2\sqrt{21}+\frac{11\sqrt{21}\,(p-22)}{21}$$

```
> B := subs(p=p0, (p-p2)/(p+p2)); C := subs(p=p0, 2*p/(p+p2));
> #approximation
```

$$B := \frac{22-\sqrt{84}}{22+\sqrt{84}}$$

$$C := \frac{44}{22+\sqrt{84}}$$

```
> psiLF := 1/sqrt(2*Pi*h^2)*int(alpha*exp(-I/h*p^2/(2*m)*t)
*exp(I*p*x), p=-infinity..infinity);
```

$$psiLF := \frac{\sqrt{2}\,e^{(\frac{1/2\,I\,(-484\,t+44\,x+440+100\,I+20\,I\,x+x^2\,I)}{1+t\,I})}}{\pi^{(1/4)}\,\sqrt{2+2\,I\,t}}$$

```
> psiLB := 1/sqrt(2*Pi*h^2)*int(B*alpha*exp(-I/h*p^2/(2*m)*t)
*exp(-I*p*x), p=-infinity..infinity);
```

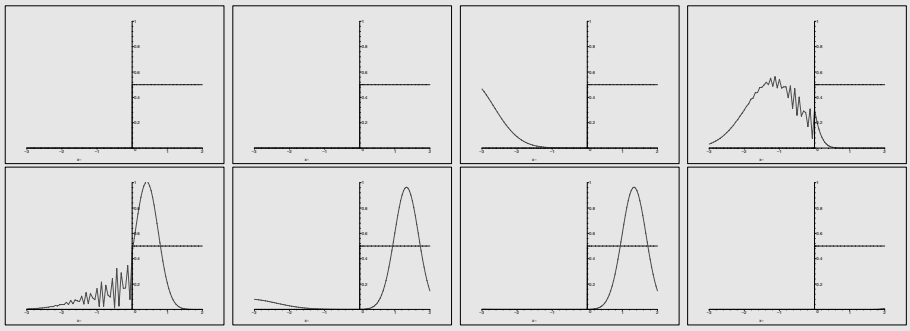
$$psiLB := -\frac{\sqrt{2}\,e^{(\frac{1/2\,I\,(-484\,t-44\,x+440+100\,I-20\,I\,x+x^2\,I)}{1+t\,I})}\,(-11+\sqrt{21})}{\pi^{(1/4)}\,(11+\sqrt{21})\,\sqrt{2+2\,I\,t}}$$

```
> psiR := 1/sqrt(2*Pi*h^2)*int(C*alpha*exp(-I/h*p^2/(2*m)*t)
*exp(I*p2appr*x), p=-infinity..infinity);
```

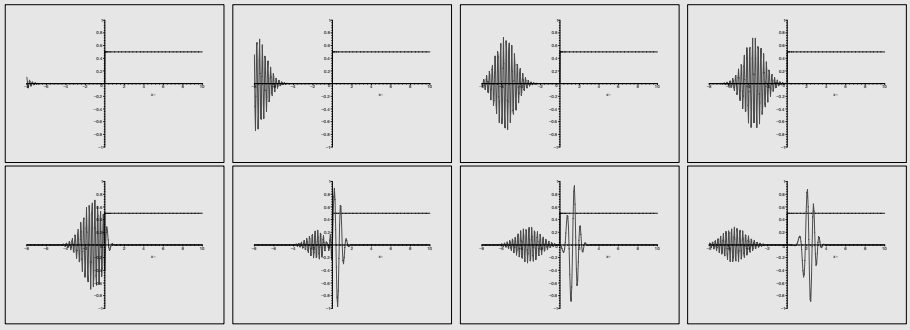
$$psiR := \frac{22\sqrt{2}\,e^{(\frac{1/42\,I\,(-10164\,t+84\,x\sqrt{21}-400\,I\,x\sqrt{21}\,t+9240+2100\,I+220\,I\,x\sqrt{21}+121\,I\,x^2)}{1+t\,I})}}{\pi^{(1/4)}\,(11+\sqrt{21})\,\sqrt{2+2\,I\,t}}$$

```
> probL := conjugate(psiLF + psiLB)*(psiLF + psiLB):
> probL := evalc(probL):
> probL := simplify(probL):
> probR := conjugate(psiR)*psiR:
> probR := evalc(probR):
> probR := simplify(probR):
> with(plots):
Warning, the name changecoords has been redefined
```

```
> pstep := plot(1/2*Heaviside(x), x=-3..2, color=blue):
> pR := animate(probR, x=0..2, t=0..0.9):
> pL := animate(probL, x=-3..0, t=0..0.9):
> display([pL, pR, pstep]);
```



```
> pstep2 := plot(1/2*Heaviside(x), x=-8..10, color=blue):
> pRwave := animate(Re(psiR), x=0..10, t=0..0.9, numpoints=150):
> pLwave := animate(Re(psiLF + psiLB), x=-8..0, t=0..0.9,
> numpoints=150):
> display([pLwave, pRwave, pstep2]);
```



Reflection of a Gaussian wave packet is commonly displayed, but less commonly calculated, in many textbooks on quantum mechanics,[1] citing the involvement of a "large amount of work on a high-speed computer." We demonstrate that, with the assistance of Maple, we can perform such a task in a straightforward manner by simply following basic formalism.

[1] A. P. French and E. F. Taylor, *An Introduction to Quantum Physics*, New York: Norton, 1978, p. 408ff; R. Eisberg and R. Resnick, *Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles*, 2nd ed., New York: Wiley, 1985, p. 192.

When Schrödinger introduced wave mechanics in 1926, the meaning of a wave function was not comprehended. Schrödinger pursued the idea of representing an electron by a wave packet, and constructed a coherent state to support his contention that waves are the only physical reality. One difficulty with his view is that, as demonstrated in the animation, a packet "diffuses" when it propagates, and it "breaks up" when it encounters a barrier. This phenomenon occurs for almost all wave packets; the coherent state, which we discuss in Section 15.8, is one of the few exceptions. In another paper submitted on June 21, 1926, Schrödinger attempted to interpret $e|\Psi|^2$ as the actual charge density, but the above-mentioned difficulty remained. Four days later, Born presented a paper on the elastic scattering of electrons by a potential barrier; his calculations indicate that waves are scattered in all directions. He abandoned the approach that relates a wave function directly to physical reality, but instead interpreted an absolute square of a wave function $|\Psi|^2$ as the *probability density*. Born's statistical view is consistent with experiment, and is adopted as the orthodox interpretation of a wave function.

Exercises

1. Verify that Schrödinger's representation of x and p satisfies the fundamental quantum condition $xp - px = i\hbar$, that is, for a function $\psi(x)$, show that

$$x\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x) - \frac{\hbar}{i}\frac{\partial}{\partial x}\left[x\psi(x)\right] = i\hbar\psi(x).$$

   Using the chain rule and the property of i, this calculation is trivial, which one can easily perform manually or with Maple.

2. For a transmission coefficient T and reflection coefficient R in the step potential in Section 14.3.1, make a plot as a function of the ratio of E to V_0.

3. For a step potential of height $V_0 = 10$ eV $= 10 \times 1.6 \times 10^{-19}$ J, solve the Schrödinger equation for (a) $E = 0.6\ V_0$; (b) $E = 1.5\ V_0$. Make graphs of the wave function and the probability density for both conditions. Observe the penetration of the wave function into the barrier for the $E < V_0$ case.

4. For an electron incident upon a barrier potential of height $V_0 = 10\,\text{eV} = 10\times1.6\times10^{-19}$ J and width 1.8×10^{-10} m, make a graph of transmission coefficient T versus total energy from $E = 0$ to $E = 10\ V_0$, which should resemble Figure 14.3.

5. Develop a worksheet for the reflection of a Gaussian wave packet by a step potential for $E_0 < V_0$. One needs only to modify the worksheet in Section 14.6.1 by altering the wave function in region 2 to

$$C\exp\left[\frac{-p_2x - iEt}{\hbar}\right],$$

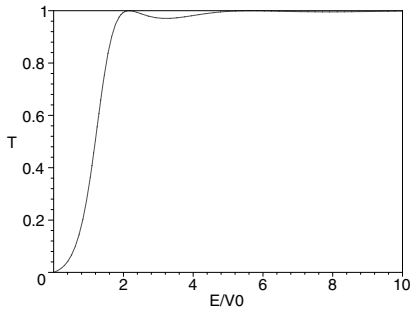


Figure 14.3: Transmission coefficient for a particle incident upon a barrier potential.

where p_2 is $\sqrt{2m(V_0 - E)}$. The coefficients B and C for the case $E < V_0$ are

$$B = \frac{ip_1 + p_2}{ip_1 - p_2}, \quad C = \frac{2ip_1}{ip_1 - p_2}.$$

6. The time-dependent Schrödinger equation is a partial differential equation, and in advanced courses one will encounter the theory of Green's functions. We are unable to treat this topic in detail, but we use the following calculation to remind the reader of the extreme usefulness of Maple. Green's function, or the *propagator*, for a free particle is (with $\hbar = 1$)

$$\langle x_b, t_b | x_a, t_a \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left\{ i \left[p(x_b - x_a) - \frac{p^2}{2m}(t_b - t_a) \right] \right\} dp; \qquad (14.61)$$

use Maple to evaluate this integral to verify that

$$\langle x_b, t_b | x_a, t_a \rangle = \left[\frac{m}{2\pi i (t_b - t_a)} \right]^{1/2} \exp\left[\frac{im(x_b - x_a)^2}{2(t_b - t_a)} \right], \quad \text{for } \frac{i(t_b - t_a)}{2m} > 0. \qquad (14.62)$$

This propagator can be interpreted as the transition amplitude for a particle to move from a space–time point (x_a, t_a) to another space–time point (x_b, t_b).

7. The standard procedure for a conservative quantum system is to set up the classical Hamiltonian, then convert it to the Schrödinger equation by replacing dynamical variables p and q with operators, see Section 14.1. In 1933, Dirac wrote a paper "The Lagrangian in Quantum Mechanics," and eight years later Feynman read it and was intrigued by a mysterious remark[2]

$$\exp\left[i \int_{t_a}^{t_b} \frac{L}{\hbar} dt \right] = \exp\left[i \frac{S(t_b, t_a)}{\hbar} \right] \quad \text{corresponds to} \quad \langle x_b, t_b | x_a, t_a \rangle.$$

[2]See the same statement in P. A. M. Dirac, *The Principles of Quantum Mechanics*, 4th ed. (rev.), Oxford: Clarendon Press, 1986, § 32, "The Action Principle," p. 128.

Dirac correctly recognized the connection between the transition amplitude and the action, but his meaning of "corresponds to" was ambiguous. Feynman deciphered the meaning of "corresponds to" as "proportional to," and in doing so he invented the space–time approach to quantum mechanics.[3] In short, Feynman's path integral is

$$\langle x_b, t_b | x_a, t_a \rangle = \sum_{\text{all paths}} A \exp\left[i \frac{S(t_b, t_a)}{\hbar} \right], \tag{14.63}$$

where A is a factor of proportionality; this path integral is equivalent to the propagator in Schrödinger's wave mechanics.

(a) The path integral is difficult to evaluate, but most paths cancel each other out except the classical trajectory. In Chapter 3, we learned that the action S is the time integral of the Lagrangian L:

$$S = \int_{t_a}^{t_b} L \, dt, \tag{14.64}$$

and, according to the principle of least action, the correct path in classical mechanics is the one that minimizes S. For a free particle in one dimension moving from point x_a at time t_a to point x_b at time t_b, verify that

$$S = \frac{m}{2} \frac{(x_b - x_a)^2}{t_b - t_a}. \tag{14.65}$$

This fact should be obvious: as a free particle must move at a constant speed at $v = \frac{x_b - x_a}{t_b - t_a}$, the time integral of $\frac{1}{2}mv^2$ gives the above result; see also equation (3.58). We see that a prefactor (which is rather difficult to calculate) multiplied by $e^{iS/\hbar}$ indeed corresponds to the propagator in the preceding problem.

(b) The path integral for a free particle is

$$\langle x, t | x_0, t_0 \rangle = \left[\frac{m}{2\pi i \hbar (t - t_0)} \right]^{1/2} \exp\left[\frac{im(x - x_0)^2}{2\hbar (t - t_0)} \right]. \tag{14.66}$$

Show that $\langle x, t | x_0, t_0 \rangle$ satisfies Schrödinger's time-dependent wave equation:

$$i\hbar \frac{\partial}{\partial t} \langle x, t | x_0, t_0 \rangle = -\left(\frac{\hbar^2}{2m} \right) \frac{\partial^2}{\partial x^2} \langle x, t | x_0, t_0 \rangle. \tag{14.67}$$

This result demonstrates the link between Feynman's Lagrangian approach of quantum mechanics and Schrödinger's wave mechanics.

[3] For a brief account, see Feynman 1965, vol. 2, p. 19-9; for an introductory treatment, see J. J. Sakurai, *Modern Quantum Mechanics*, Reading, MA: Addison-Wesley, 1994, p. 109ff.

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15 Schrödinger Equation in One Dimension (II): Bound States

Continuing our discussion of the Schrödinger equation in one dimension, in this chapter we treat bound states, for which a particle is confined to space in a particular region. For a piecewise-constant potential, the technique of solving the Schrödinger equation is the same as that in the preceding chapter, namely matching coefficients by imposing required continuity conditions at the boundaries. We then discuss several notable problems, including the quantum-mechanical harmonic oscillator and the Morse oscillator. These problems involve second-order ordinary differential equations; their solutions are well established special functions, and essentially all of them are defined in Maple.[1] We also discuss the time evolution of the wave functions for nonstationary states.

15.1 Discrete Spectrum

We briefly review what we have learned in the previous chapter: a quantum state that has definite energy is a stationary state, and the spatial part of the corresponding wave function satisfies the time-independent Schrödinger equation,

$$\boxed{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x)}; \tag{15.1}$$

the complete wave function is the product of the spatial and temporal parts,

$$\Psi(x,t)=\psi(x)e^{-iEt/\hbar}. \tag{15.2}$$

For a bound state, for which the particle is confined to space in a particular region, the total energy is less than the maximum of the potential energy,

$$E<\lim_{|x|\to\infty}V(x). \tag{15.3}$$

In addition to the general requirements that the wave function $\psi(x)$ and its derivative $\frac{d\psi(x)}{dx}$ must be continuous, for a bound state we must ensure that the wave function vanishes at

[1] With a proper interpretation of the Maple (version 8 or higher) output, we may directly solve a Schrödinger equation and determine the discrete energy levels; see Appendix B.2.

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$x = \pm\infty$ by imposing a condition that

$$\psi(x) \to 0 \text{ as } |x| \to \infty, \tag{15.4}$$

so that the wave function $\psi(x)$ remains finite everywhere. The most remarkable consequence of the Schrödinger equation is that these requirements yield discrete energies E. Quantization of energy is an inevitable result arising purely from the property of the differential equation. We will examine several examples in this chapter which manifest this astonishing property.

15.2 Infinite Potential Well

A particle is confined to a line segment between infinite barriers; the corresponding potential energy for this infinitely deep well, sometimes called a rigid potential well, is defined by a discontinuous function,

$$V(x) = \begin{cases} \infty, & x < 0 \text{ or } x > a, \\ 0, & 0 < x < a. \end{cases} \tag{15.5}$$

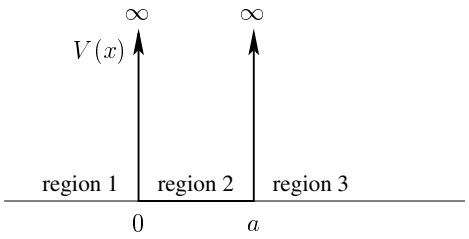


Figure 15.1: Infinite potential well.

We denote regions with $x < 0$, $0 < x < a$ and $x > a$ as 1, 2 and 3 respectively; see Figure 15.1. Because $V = \infty$ in regions 1 and 3, the wave function must be zero there,

$$\begin{aligned} \psi_1(x) &= 0, \quad x < 0, \\ \psi_3(x) &= 0, \quad x > a. \end{aligned} \tag{15.6}$$

In region 2, the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x). \tag{15.7}$$

This problem is the same as the zero-potential problem in Section 14.2. However, instead of writing the general solution as $e^{\pm ikx}$, we invoke Euler's formula and express the solution in the form

$$\psi_2(x) = A\cos(kx) + B\sin(kx). \tag{15.8}$$

When we treat unbound states, it is convenient to write a wave function as $e^{\pm ikx}$, which signifies a traveling wave; in contrast, for a bound state we prefer to write a wave function as $\sin(kx)$ and $\cos(kx)$, which signify standing waves.

Substituting $\psi_2(x)$ directly into the Schrödinger equation, we obtain

$$E = \frac{\hbar^2 k^2}{2m}. \tag{15.9}$$

Applying the continuity requirement at $x = 0$, we reject the cosine solution,

$$\psi_1(0) = \psi_2(0), \quad A = 0. \tag{15.10}$$

At $x = a$,

$$B\sin(ka) = 0, \quad ka = n\pi \text{ for } n = 1, 2, 3, \ldots. \tag{15.11}$$

Because k can only take particular values, namely $n\pi/a$, to satisfy the requirement of the wave function, the energy E becomes quantized:

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2ma^2}. \tag{15.12}$$

Although $\psi(x)$ must be continuous, because for this problem there is an abrupt increase of potential from 0 to infinity at $x = 0$ and $x = a$, the continuity requirement of $\psi'(x)$ is inapplicable. Unlike problems that we discussed in the previous chapter in which a wave function exponentially decays in a region $E < V_0$, because in this problem $V_0 = \infty$, the wave function must directly vanish at the boundaries.

Worksheet 15.1 In this worksheet we use `h` for $\hbar$. Maple directly solves the Schrödinger equation without invoking the wave number k. Imposing the continuity conditions at the boundaries, we obtain discrete energies. By setting Maple's environmental variable `_EnvAllSolutions` to be `true`, we force the `solve` command to return solutions of the sine function in complete sets; see help under `solve` for further information. The symbol $_Z1$ in the output of `Soln2` represents an integer.

```
> Eq1 := -h/(2*m)*diff(psi(x), x$2) = En*psi(x);
```

$$Eq1 := -\frac{1}{2}\frac{h\left(\frac{d^2}{dx^2}\psi(x)\right)}{m} = En\,\psi(x)$$

```
> Soln1 := dsolve(Eq1, psi(x));
```

$$Soln1 := \psi(x) = _C1 \sin\left(\frac{\sqrt{2}\sqrt{En}\sqrt{m}\,x}{\sqrt{h}}\right) + _C2 \cos\left(\frac{\sqrt{2}\sqrt{En}\sqrt{m}\,x}{\sqrt{h}}\right)$$

```
> assign(Soln1);
> Eq3 := eval(psi(x), x=0) = 0;
```

$$Eq3 := _C2 = 0$$

```
> Eq4 := eval(psi(x), {x=a,Eq3}) = 0;
```

$$Eq4 := _C1 \sin\left(\frac{\sqrt{2}\,\sqrt{En}\,\sqrt{m}\,a}{\sqrt{h}}\right) = 0$$

```
> _EnvAllSolutions := true:
> Soln2 := solve({Eq4}, En);
```

$$Soln2 := \left\{En = \frac{\pi^2 _Z1^2\, h}{2\,m\,a^2}\right\}$$

15.3 Finite Potential Well

Before solving another quantum-mechanical problem, we comment on the symmetry properties that enable us to abbreviate calculations. If the potential-energy function is even, such that $V(x) = V(-x)$, the Schrödinger equation is unaltered when the sign of the coordinate is reversed. Hence if $\psi(x)$ is a solution, $\psi(-x)$ is also a solution. We relate these two wave functions through a constant $\psi(-x) = c\psi(x)$. Reversing the sign of x again we obtain $\psi(x) = c^2\psi(x)$; therefore $c = \pm 1$. We conclude that for a symmetric potential the wave functions must be either even, for which $\psi(-x) = \psi(x)$, or odd, for which $\psi(-x) = -\psi(x)$. We present the following example to illustrate the usefulness of symmetry properties.

For a well of finite depth V_0 as a model for the potential energy, the suitable defining function is

$$V(x) = \begin{cases} V_0, & x < -a/2 \text{ or } x > a/2, \\ 0, & -a/2 < x < a/2. \end{cases} \tag{15.13}$$

This function resembles that of an infinitely deep potential well in the preceding section except that V_0 is finite. In order to take advantage of the symmetry property, we choose our coordinate so that $V(x) = V(-x)$. Again we divide the one-dimensional space into regions 1, 2 and 3, corresponding to $x < -a/2$, $-a/2 < x < a/2$ and $x > a/2$, respectively. The wave functions take the form

$$\begin{cases} \psi_1(x) = Ae^{\kappa_2 x}, & x < -a/2, \\ \psi_2(x) = B_1 \sin(k_1 x) + B_2 \cos(k_1 x), & -\frac{a}{2} < x < \frac{a}{2}, \\ \psi_3(x) = Ce^{-\kappa_2 x}, & x > a/2, \end{cases} \tag{15.14}$$

where again

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, \quad \kappa_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}; \tag{15.15}$$

see Section 14.3.2. Applying continuity conditions at the boundaries, we have

$$\psi_1(-a/2) = \psi_2(-a/2), \quad Ae^{-\kappa_2 a/2} = -B_1 \sin(k_1 a/2) + B_2 \cos(k_1 a/2), \tag{15.16a}$$

$$\psi_2(a/2) = \psi_3(a/2), \quad B_1 \sin(k_1 a/2) + B_2 \cos(k_1 a/2) = Ce^{-\kappa_2 a/2}, \tag{15.16b}$$

$$\psi_1'(-a/2) = \psi_2'(-a/2), \quad A\kappa_2 e^{-\kappa_2 a/2} = B_1 k_1 \cos(k_1 a/2) + B_2 k_1 \sin(k_1 a/2), \tag{15.16c}$$

$$\psi_2'(a/2) = \psi_3'(a/2), \quad B_1 k_1 \cos(k_1 a/2) - B_2 k_1 \sin(k_1 a/2) = -C\kappa_2 e^{-\kappa_2 a/2}. \tag{15.16d}$$

As the potential is symmetric, namely $V(x) = V(-x)$, $\psi(x)$ must be either even or odd. We thus classify the solutions as symmetric or antisymmetric, and discuss them separately.

1. Symmetric function
   For a symmetric solution, A must equal C, and B_1 must be zero: we reject the $\sin(k_1 x)$ term. The four equations in (15.16) reduce to two independent ones,

   $$Ae^{-\kappa_2 a/2} = B_2 \cos(k_1 a/2), \tag{15.17a}$$

   and

   $$A\kappa_2 e^{-\kappa_2 a/2} = B_2 k_1 \sin(k_1 a/2). \tag{15.17b}$$

   Dividing equation (15.17b) by (15.17a), we have

   $$\tan(k_1 a/2) = \frac{\kappa_2}{k_1}. \tag{15.18}$$

   Equation (15.18) is a transcendental equation, the roots of which determine the accessible energies E. Only particular discrete values of E satisfy this equation, which is evidence of the quantization of energy for a bound state. These values can be found graphically and numerically, which Maple is able to perform.

   After we have found a particular energy E, we can calculate k_1 and κ_2, and substitute them back into either equation (15.17a) or (15.17b) to relate A and B_2. Because $C = A$ and $B_1 = 0$, we obtain the wave function for this energy state. In the customary manner, we evaluate A, which is so far arbitrary, by imposing a normalization condition,

   $$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)\, dx = 1. \tag{15.19}$$

2. Antisymmetric function
   For an antisymmetric solution, A must equal $-C$, and B_2 must be zero: we reject the $\cos(k_1 x)$ term. The four equations in (15.16) reduce to two independent ones,

   $$Ae^{-\kappa_2 a/2} = -B_1 \sin(k_1 a/2), \tag{15.20a}$$

   and

   $$A\kappa_2 e^{-\kappa_2 a/2} = B_1 k_1 \cos(k_1 a/2). \tag{15.20b}$$

Dividing equation (15.20b) by (15.20a), we obtain

$$\cot(k_1 a/2) = -\frac{\kappa_2}{k_1}. \tag{15.21}$$

We again find a transcendental equation (15.21), for which we must employ graphical and numerical methods to evaluate values of the discrete energies for this class of solution. Once an energy is determined, either equation (15.20a) or (15.20b) provides a relation between A and B_1. In this case, $C = -A$ and $B_2 = 0$, and we obtain the wave function for this state.

Example 15.1 This numerical example serves to illustrate the graphical and numerical methods. Suppose that we have an electron subject to potential energy of a finite well, for which $a = 1.8 \times 10^{-10}$ m and $V_0 = 64$ eV $= 64 \times 1.6 \times 10^{-19}$ J. Find possible energies for $E < V_0$, and sketch the corresponding wave functions.

Solution We have

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, \quad \kappa_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}.$$

For a symmetric wave function, the energies are evaluated from

$$\tan(k_1 a/2) = \frac{\kappa_2}{k_1};$$

for antisymmetric ones,

$$\cot(k_1 a/2) = -\frac{\kappa_2}{k_1}.$$

We plot $\tan(k_1 a/2)$ or $\cot(k_1 a/2)$, and κ_2/k_1 or $-\kappa_2/k_1$, respectively, as a function of E; intersections of these two curves represent allowed energies. From these plots we find two roots for symmetric wave functions,

$$E_1 = 1.05 \times 10^{-18} \text{ J}, \quad E_3 = 8.58 \times 10^{-18} \text{ J},$$

and one root for the antisymmetric wave function,

$$E_2 = 4.09 \times 10^{-18} \text{ J}.$$

After obtaining the energy, we can evaluate the coefficients of the corresponding wave function.

Worksheet 15.2 We define the wave function in three regions, and impose continuity conditions in `Eq1` through `Eq4`. For a symmetric function, we set `B1 := 0` and `C := A`; we obtain a transcendental equation `Eq13`, which determines the discrete energies. For an antisymmetric function, `B2 := 0` and `C := -A`, and the rest is analogous to the symmetric case. We plot each side of the transcendental equation to locate the intersections of the curves, and invoke the `fsolve` command to find the root. Once a specific energy has been found, we evaluate the coefficients for the corresponding state. Apostrophes serve to "unassign" the variables, so that we can evaluate coefficients for another state using the original `Eq1`. When we plot the wave functions, instead of normalizing to determine `A`, we choose an arbitrary value of this parameter which is convenient for visual presentation. Again `h` is $\hbar$.

```
> psi1 := x -> A*exp(kappa2*x);
```

$$\psi 1 := x \to A\, e^{(\kappa 2\, x)}$$

```
> psi2 := x -> B1*sin(k1*x) + B2*cos(k1*x);
```

$$\psi 2 := x \to B1 \sin(k1\, x) + B2 \cos(k1\, x)$$

```
> psi3 := x -> C*exp(-kappa2*x);
```

$$\psi 3 := x \to C\, e^{(-\kappa 2\, x)}$$

```
> Eq1 := psi1(-a/2) = psi2(-a/2);
```

$$Eq1 := A\, e^{(-\frac{\kappa 2\, a}{2})} = -B1 \sin\left(\frac{k1\, a}{2}\right) + B2 \cos\left(\frac{k1\, a}{2}\right)$$

```
> Eq2 := psi2(a/2) = psi3(a/2);
```

$$Eq2 := B1 \sin\left(\frac{k1\, a}{2}\right) + B2 \cos\left(\frac{k1\, a}{2}\right) = C\, e^{(-\frac{\kappa 2\, a}{2})}$$

```
> Eq3 := D(psi1)(-a/2) = D(psi2)(-a/2);
```

$$Eq3 := A\, \kappa 2\, e^{(-\frac{\kappa 2\, a}{2})} = B1 \cos\left(\frac{k1\, a}{2}\right) k1 + B2 \sin\left(\frac{k1\, a}{2}\right) k1$$

```
> Eq4 := D(psi2)(a/2) = D(psi3)(a/2);
```

$$Eq4 := B1 \cos\left(\frac{k1\, a}{2}\right) k1 - B2 \sin\left(\frac{k1\, a}{2}\right) k1 = -C\, \kappa 2\, e^{(-\frac{\kappa 2\, a}{2})}$$

```
> B1 := 0; C := A;
```

$$B1 := 0$$
$$C := A$$

```
> Eq1; Eq2; Eq3; Eq4;
```

$$A\, e^{(-\frac{\kappa 2\, a}{2})} = B2 \cos\left(\frac{k1\, a}{2}\right)$$

$$B2 \cos\left(\frac{k1\, a}{2}\right) = A\, e^{(-\frac{\kappa 2\, a}{2})}$$

$$A\, \kappa 2\, e^{(-\frac{\kappa 2\, a}{2})} = B2 \sin\left(\frac{k1\, a}{2}\right) k1$$

$$-B2 \sin\left(\frac{k1\, a}{2}\right) k1 = -A\, \kappa 2\, e^{(-\frac{\kappa 2\, a}{2})}$$

```
> Eq11 := isolate(Eq1, cos(1/2*k1*a));
```

$$Eq11 := \cos\left(\frac{k1\, a}{2}\right) = \frac{A\, e^{(-\frac{\kappa 2\, a}{2})}}{B2}$$

```
> Eq12 := isolate(Eq3, sin(1/2*k1*a));
```

$$Eq12 := \sin\left(\frac{k1\, a}{2}\right) = \frac{A\, \kappa 2\, e^{(-\frac{\kappa 2\, a}{2})}}{B2\, k1}$$

```
> Eq13 := lhs(Eq12)/lhs(Eq11) = rhs(Eq12)/rhs(Eq11);
```

$$Eq13 := \frac{\sin\left(\frac{k1\,a}{2}\right)}{\cos\left(\frac{k1\,a}{2}\right)} = \frac{\kappa 2}{k1}$$

```
> A := 'A': B1 := 'B1':  B2 := 'B2':  C := 'C':
> B2 := 0; C := -A;
```

$$B2 := 0$$
$$C := -A$$

```
> Eq1; Eq2; Eq3; Eq4;
```

$$A\,e^{(-\frac{\kappa 2\,a}{2})} = -B1\sin\left(\frac{k1\,a}{2}\right)$$

$$B1\sin\left(\frac{k1\,a}{2}\right) = -A\,e^{(-\frac{\kappa 2\,a}{2})}$$

$$A\,\kappa 2\,e^{(-\frac{\kappa 2\,a}{2})} = B1\cos\left(\frac{k1\,a}{2}\right)k1$$

$$B1\cos\left(\frac{k1\,a}{2}\right)k1 = A\,\kappa 2\,e^{(-\frac{\kappa 2\,a}{2})}$$

```
> Eq21 := isolate(Eq1, sin(1/2*k1*a));
```

$$Eq21 := \sin\left(\frac{k1\,a}{2}\right) = -\frac{A\,e^{(-\frac{\kappa 2\,a}{2})}}{B1}$$

```
> Eq22 := isolate(Eq3, cos(1/2*k1*a));
```

$$Eq22 := \cos\left(\frac{k1\,a}{2}\right) = \frac{A\,\kappa 2\,e^{(-\frac{\kappa 2\,a}{2})}}{B1\,k1}$$

```
> Eq23 := lhs(Eq21)/lhs(Eq22) = rhs(Eq21)/rhs(Eq22);
```

$$Eq23 := \frac{\sin\left(\frac{k1\,a}{2}\right)}{\cos\left(\frac{k1\,a}{2}\right)} = -\frac{k1}{\kappa 2}$$

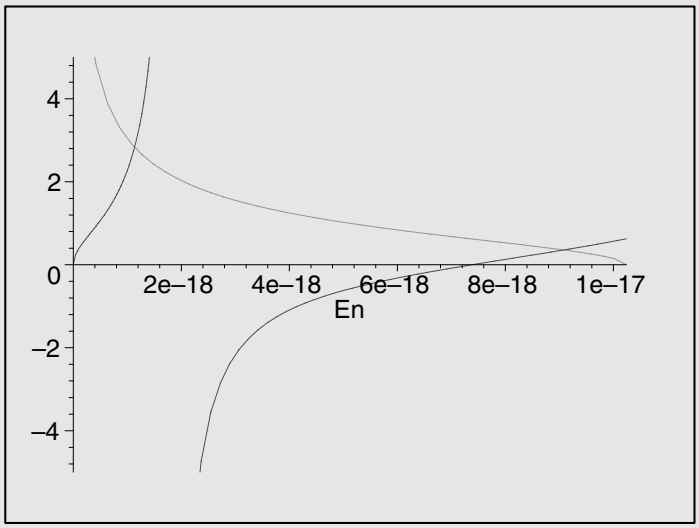
```
> a := 1.8e-10; V0 := 64*1.6e-19; h := 1.055e-34:  m := 9.1e-31:
```

$$a := 0.18\,10^{-9}$$
$$V0 := 0.1024\,10^{-16}$$

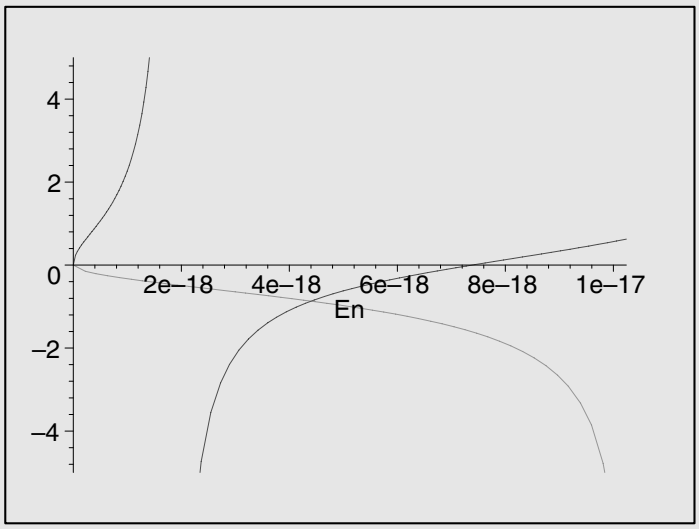
```
> k1 := sqrt(2*m*En)/h; kappa2 := sqrt(2*m*(V0 - En))/h;
```

$$k1 := 0.1278742897\,10^{20}\sqrt{En}$$
$$\kappa 2 := 0.9478672986\,10^{34}\sqrt{0.186368\,10^{-46} - 0.182\,10^{-29}\,En}$$

```
> plot([lhs(Eq13), rhs(Eq13)], En=0..V0, -5..5, discont=true);
```




```
> plot([lhs(Eq23), rhs(Eq23)], En=0..V0, -5..5, discont=true);
```




```
> En1 := fsolve(Eq13, En=0..2e-18);
```

$$En1 := 0.1142627411\,10^{-17}$$

```
> En2 := fsolve(Eq23, En=2e-18..6e-18);
```

$$En2 := 0.4433992489\,10^{-17}$$

```
> En3 := fsolve(Eq13, En=8e-18..1e-17);
```

$$En3 := 0.9128959534\,10^{-17}$$

```
> A := 'A': B1 := 'B1':  B2 := 'B2':  C := 'C': En := En1;
```

$$En := 0.1142627411\,10^{-17}$$

```
> A := 10*En; B1 := 0; C := A;
```

$$A := 0.1142627411\,10^{-16}$$

$$B1 := 0$$

$$C := 0.1142627411\,10^{-16}$$

```
> Eq41 := Eq1;
```

$$Eq41 := 0.3551136851\,10^{-18} = 0.3340429735\,B2$$

```
> Eq42 := isolate(Eq41, B2);
```

$$Eq42 := B2 = 0.1063077847\,10^{-17}$$

```
> assign(Eq42);
> p1s1 := plot(psi1(x) + En, x=-a..-a/2):
> p1s2 := plot(psi2(x) + En, x=-a/2..a/2):
> p1s3 := plot(psi3(x) + En, x=a/2..a):
> A := 'A': B1 := 'B1':  B2 := 'B2':  C := 'C': En := En2;
```

$$En := 0.4433992489\,10^{-17}$$

```
> A := 5*En; B2 := 0; C := -A;
```

$$A := 0.2216996244\,10^{-16}$$

$$B2 := 0$$

$$C := -0.2216996244\,10^{-16}$$

```
> Eq51 := Eq1;
```

$$Eq51 := 0.1384923154\,10^{-17} = -0.6580327348\,B1$$

```
> Eq52 := isolate(Eq51, B1);
```

$$Eq52 := B1 = -0.2104641731\,10^{-17}$$

```
> assign(Eq52);
> p2a1 := plot(psi1(x) + En, x=-a..-a/2):
> p2a2 := plot(psi2(x) + En, x=-a/2..a/2):
> p2a3 := plot(psi3(x) + En, x=a/2..a):
> A := 'A': B1 := 'B1':  B2 := 'B2':  C := 'C': En := En3;
```

$$En := 0.9128959534\,10^{-17}$$

```
> A := En/2; B1 := 0; C := A;
```

$$A := 0.4564479767\,10^{-17}$$

$$B1 := 0$$

$$C := 0.4564479767\,10^{-17}$$

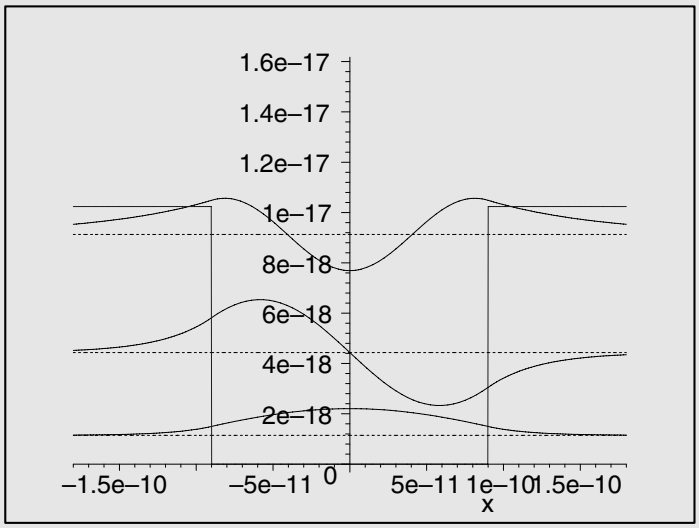
```
> Eq61 := Eq1;
```

$$Eq61 := 0.1356924962\,10^{-17} = -0.9441927538\,B2$$

```
> Eq62 := isolate(Eq61, B2);
```

$$Eq62 := B2 = -0.1437127066\,10^{-17}$$

```
> assign(Eq62);
> p3s1 := plot(psi1(x) + En, x=-a..-a/2):
> p3s2 := plot(psi2(x) + En, x=-a/2..a/2):
> p3s3 := plot(psi3(x) + En, x=a/2..a):
> Vx := piecewise(x>-a/2 and x<a/2, 0, x>a/2, V0, x<-a/2, V0):
> ppot := plot(Vx, x=-a..a, color=blue):
> pEn := plot([En1, En2, En3], x=-a..a):
> with(plots):
Warning, the name changecoords has been redefined
> display([ppot, pEn, p1s1, p1s2, p1s3, p2a1, p2a2, p2a3, p3s1,
> p3s2, p3s3]);
```



In the plot we observe penetration of the wave function into classically forbidden regions for which $E < V_0$.

15.4 Series Solution and Hermite Equation

The quantum-mechanical treatment of the harmonic oscillator involves the Hermite equation,

$$\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + 2\lambda y = 0. \tag{15.22}$$

Before discussing the physics, we digress to solve this equation.

We apply the method of series solution, which is further discussed in Appendix B.1. Let the solution take the form of an infinite series,

$$y = \sum_{k=0}^{\infty} a_k x^k; \tag{15.23}$$

we find the first and second derivatives,

$$\frac{dy}{dx} = \sum_{k=1}^{\infty} k a_k x^{k-1}, \quad \frac{d^2y}{dx^2} = \sum_{k=2}^{\infty} k(k-1) a_k x^{k-2}. \tag{15.24}$$

Substituting equations (15.23) and (15.24) into equation (15.22), we produce

$$\sum_{k=2}^{\infty} k(k-1) a_k x^{k-2} - \sum_{k=1}^{\infty} 2k a_k x^k + \sum_{k=0}^{\infty} 2\lambda a_k x^k = 0. \tag{15.25}$$

We shift the index of summation in the first term by changing $k \to k+2$,

$$\sum_{k=0}^{\infty} (k+2)(k+1) a_{k+2} x^k - \sum_{k=1}^{\infty} 2k a_k x^k + \sum_{k=0}^{\infty} 2\lambda a_k x^k = 0. \tag{15.26}$$

Collecting coefficients of the same degree, we obtain a recurrence relation for $k \geq 1$,

$$a_{k+2} = \frac{-2\lambda + 2k}{(k+2)(k+1)} a_k. \tag{15.27}$$

Worksheet 15.3 In performing the above manipulations with Maple, it is sufficient to work with five consecutive terms. To collect coefficients of the same degree, we employ the `coeff` command.

```
> y := sum(a[i]*x^i, i=k-2..k+2);
```

$$y := a_{k-2}\, x^{(k-2)} + a_{-1+k}\, x^{(-1+k)} + a_k\, x^k + a_{1+k}\, x^{(1+k)} + a_{k+2}\, x^{(k+2)}$$

```
> EqH := diff(y,x$2) - 2*x*diff(y,x) + 2*lambda*y = 0:
```

```
> Eq1 := simplify(EqH);
```

$$Eq1 := -2\,a_{1+k}\,x^{(1+k)} + 4\,a_{k-2}\,x^{(k-2)} + 2\,a_{-1+k}\,x^{(-1+k)} - 4\,a_{k+2}\,x^{(k+2)} - a_k\,x^{(k-2)}\,k + a_k\,x^{(k-2)}\,k^2 - 5\,a_{k-2}\,x^{(k-4)}\,k + 2\,\lambda\,a_{1+k}\,x^{(1+k)} + a_{k-2}\,x^{(k-4)}\,k^2 + a_{-1+k}\,x^{(-3+k)}\,k^2 - 3\,a_{-1+k}\,x^{(-3+k)}\,k + a_{1+k}\,x^{(-1+k)}\,k^2 + a_{1+k}\,x^{(-1+k)}\,k + a_{k+2}\,x^k\,k^2 + 3\,a_{k+2}\,x^k\,k + 2\,\lambda\,a_{k-2}\,x^{(k-2)} + 2\,\lambda\,a_{-1+k}\,x^{(-1+k)} + 2\,\lambda\,a_k\,x^k + 2\,\lambda\,a_{k+2}\,x^{(k+2)} + 6\,a_{k-2}\,x^{(k-4)} + 2\,a_{-1+k}\,x^{(-3+k)} + 2\,a_{k+2}\,x^k - 2\,x^{(k-2)}\,a_{k-2}\,k - 2\,x^{(-1+k)}\,a_{-1+k}\,k - 2\,x^{(1+k)}\,a_{1+k}\,k - 2\,x^{(k+2)}\,a_{k+2}\,k - 2\,x^k\,a_k\,k = 0$$

```
> Eq2 := map(coeff,Eq1,x^k);
```

$$Eq2 := a_{k+2}\,k^2 + 3\,a_{k+2}\,k + 2\,\lambda\,a_k - 2\,a_k\,k + 2\,a_{k+2} = 0$$

```
> Eq3 := isolate(Eq2,a[k+2]);
```

$$Eq3 := a_{k+2} = \frac{-2\,\lambda\,a_k + 2\,a_k\,k}{k^2 + 3\,k + 2}$$

```
> Eq4 := factor(Eq3);
```

$$Eq4 := a_{k+2} = \frac{2\,a_k\,(-\lambda + k)}{(k+2)\,(1+k)}$$

Because we have a recurrence relation between a_{k+2} and a_k, we have an even series with coefficients $a_0, a_2, a_4, \ldots$, and an odd series with coefficients $a_1, a_3, a_5, \ldots$. Explicitly, if we set $a_0 = 1$, we obtain the even solution,

$$y_1 = 1 - \frac{2\lambda}{2!}x^2 + \frac{2^2\lambda(\lambda-2)}{4!}x^4 - \frac{2^3\lambda(\lambda-2)(\lambda-4)}{6!}x^6 + \ldots; \tag{15.28}$$

analogously if we set $a_1 = 1$, we obtain the odd solution,

$$y_2 = x - \frac{2(\lambda-1)}{3!}x^3 + \frac{2^2(\lambda-1)(\lambda-3)}{5!}x^5 - \frac{2^3(\lambda-1)(\lambda-3)(\lambda-5)}{7!}x^7 + \ldots. \tag{15.29}$$

From the recurrence relation, or from the above two equations, we notice that only when $\lambda = 0, 1, 2, 3, 4, 5, \ldots$ does the series terminate at the x^λ term. For example, if $\lambda = 5$,

$$y = x - \frac{4}{3}x^3 + \frac{4}{15}x^5;$$

if $\lambda = 6$,

$$y = 1 - 6x^2 + 4x^4 - \frac{8}{15}x^6.$$

Hence when λ is zero or a positive integer, $y \to 0$ as $x \to \infty$. These solutions that correspond to the Hermite equation where λ is zero or a positive integer are called the Hermite polynomials.

15.5 Linear Harmonic Oscillator

We discuss the harmonic oscillator that appears in many applications of quantum mechanics as a basic model. For instance, it serves as the potential-energy function of a diatomic molecule of which two nuclei are near their equilibrium separation. In terms of the variable x which measures the displacement from the equilibrium position, the potential energy for this problem is

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2. \tag{15.30}$$

The Schrödinger equation for such an oscillator is then

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi. \tag{15.31}$$

To solve this problem, we first eliminate all excess constants such as m, $\hbar$, by introducing a dimensionless variable ξ,

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x. \tag{15.32}$$

Maple can assist us to determine such a dimensionless variable; see both Appendix B.2 and an example in Section 15.6. With this parameter, we obtain a dimensionless equation,

$$\frac{d^2\psi}{d\xi^2} + \left[\left(\frac{2E}{\hbar\omega}\right) - \xi^2\right]\psi = 0, \tag{15.33}$$

which simplifies algebraic manipulation. We further simplify this equation: examining equation (15.33), for large ξ we can neglect $2E/\hbar\omega$ in comparison with ξ^2. The equation $\psi'' = \xi^2\psi$ has an asymptotic solution $\psi = e^{-\xi^2/2}$. Defining

$$\psi = e^{-\xi^2/2}\chi(\xi), \tag{15.34}$$

and substituting it into equation (15.33), we have

$$\frac{d^2\chi}{d\xi^2} - 2\xi\frac{d\chi}{d\xi} + \left(\frac{2E}{\hbar\omega} - 1\right)\chi = 0, \tag{15.35}$$

which is the Hermite equation, discussed in the preceding section. With the definition

$$\frac{2E}{\hbar\omega} - 1 = 2\lambda, \tag{15.36}$$

for the wave function $\psi(x)$ to be square integrable for all x, λ must be zero or a positive integer. This property yields a quantization of energy,

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, 3, \ldots. \tag{15.37}$$

Even for $n = 0$, denoting the state of least energy accessible to this oscillator, the energy is not zero but $\frac{1}{2}\hbar\omega$, and is called the residual or zero-point energy.

The problem of the quantum-mechanical harmonic oscillator is thus solved. The discrete energies are specified in equation (15.37); the normalized wave functions are

$$\psi_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-m\omega x^2/2\hbar} H_n\left(x\sqrt{m\omega/\hbar}\right). \tag{15.38}$$

Avoid confusion of the symbols that we employ. In preceding examples with a piecewise-constant potential, the subscript n in $\psi_n(x)$ serves to indicate separate regions of space, but here n is a quantum number of a state of discrete energy. Although we offer no derivation of the normalization factor one can, in a practical manner, use Maple to find it by integrating the square of any unnormalized wave function.

Worksheet 15.4 Hermite polynomials are defined as `HermiteH` in Maple. In this worksheet we plot the energies and normalized wave functions.

```
> psi := (n,xi) ->
> (2^n*factorial(n))^(-1/2)*exp(-xi^2/2)*HermiteH(n,xi);
```

$$\psi := (n, \xi) \to \frac{e^{(-1/2\,\xi^2)}\,\mathrm{HermiteH}(n, \xi)}{\sqrt{2^n\,n!}}$$

```
> expand(psi(0, xi));
```

$$e^{(-\frac{\xi^2}{2})}$$

```
> expand(psi(1, xi));
```

$$\sqrt{2}\,e^{(-\frac{\xi^2}{2})}\,\xi$$

```
> expand(psi(2, xi));
```

$$-\frac{1}{4}\sqrt{8}\,e^{(-\frac{\xi^2}{2})} + \frac{1}{2}\sqrt{8}\,e^{(-\frac{\xi^2}{2})}\,\xi^2$$

```
> expand(psi(3, xi));
```

$$\frac{1}{6}\sqrt{48}\,e^{(-\frac{\xi^2}{2})}\,\xi^3 - \frac{1}{4}\sqrt{48}\,e^{(-\frac{\xi^2}{2})}\,\xi$$

```
> expand(psi(4, xi));
```

$$\frac{1}{32}\sqrt{384}\,e^{(-\frac{\xi^2}{2})} + \frac{1}{24}\sqrt{384}\,e^{(-\frac{\xi^2}{2})}\,\xi^4 - \frac{1}{8}\sqrt{384}\,e^{(-\frac{\xi^2}{2})}\,\xi^2$$

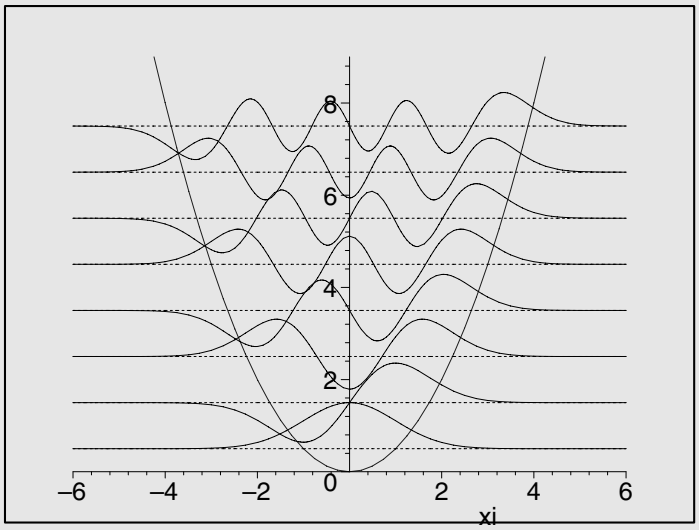
```
> expand(psi(5, xi));
```

$$\frac{1}{120}\sqrt{3840}\,e^{(-\frac{\xi^2}{2})}\,\xi^5 - \frac{1}{24}\sqrt{3840}\,e^{(-\frac{\xi^2}{2})}\,\xi^3 + \frac{1}{32}\sqrt{3840}\,e^{(-\frac{\xi^2}{2})}\,\xi$$

```
> expand(psi(6, xi));
```

$$-\frac{1}{384}\sqrt{46080}\,e^{(-\frac{\xi^2}{2})} + \frac{1}{720}\sqrt{46080}\,e^{(-\frac{\xi^2}{2})}\,\xi^6 - \frac{1}{96}\sqrt{46080}\,e^{(-\frac{\xi^2}{2})}\,\xi^4 + \frac{1}{64}\sqrt{46080}\,e^{(-\frac{\xi^2}{2})}\,\xi^2$$

```
> plot([psi(0,xi)+ 1/2, 1/2, psi(1,xi) + 3/2, 3/2, psi(2,xi)+ 5/2,
> 5/2, psi(3,xi) + 7/2, 7/2, psi(4,xi) + 9/2, 9/2, psi(5,xi)
> + 11/2,  11/2, psi(6,xi) + 13/2, 13/2, psi(7,xi) + 15/2, 15/2,
> psi(18,xi) + 37/2, 37/2, xi^2/2], xi=-6..6, 0..9);
```



We list the first six wave functions for the harmonic oscillator in Table 15.1. Solutions appear in two classes – symmetric and antisymmetric wave functions; this feature is consistent with the symmetric nature of the potential energy, because $V(x) = V(-x)$.

Table 15.1: The first six wave functions for harmonic oscillator with variable $\xi = \sqrt{(m\omega/\hbar)}\, x$.

n	$\psi_n/(m\omega/\pi\hbar)^{1/4}$
0	$e^{-\xi^2/2}$
1	$\sqrt{2}e^{-\xi^2/2}(2\xi)$
2	$\frac{1}{\sqrt{2}}e^{-\xi^2/2}(2\xi^2-1)$
3	$\frac{1}{\sqrt{3}}e^{-\xi^2/2}(2\xi^3-3\xi)$
4	$\frac{1}{\sqrt{24}}e^{-\xi^2/2}(4\xi^4-12\xi^2+3)$
5	$\frac{1}{\sqrt{60}}e^{-\xi^2/2}(4\xi^5-20\xi^3+15\xi)$

15.6 Homogeneous Field

We consider this function for the potential energy,

$$V(x) = F|x|, \tag{15.39}$$

which might represent the case of a particle subject to a constant force F. This potential serves as an excellent model for a quark and an antiquark in a bound system.[2] The Schrödinger equation for this problem is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + F|x|\psi = E\psi. \tag{15.40}$$

Because $V(x) = V(-x)$, we take advantage of the symmetry property discussed in Section 15.3. We only need to consider the space $x < 0$, and then construct the other half-space based on the symmetry property. Using Maple to solve this Schrödinger equation directly, we obtain the solution as an Airy function.

Worksheet 15.5 Airy functions are defined as `AiryAi` in Maple. Another class of solution in `AiryBi(x)` that fails to converge at large x is inappropriate for our purpose. We use the symbol `h_` for $\hbar$.

```
> Eq1 := -h_^2/(2*m)*diff(psi(x), x$2) - F*x*psi(x) = En*psi(x);
```

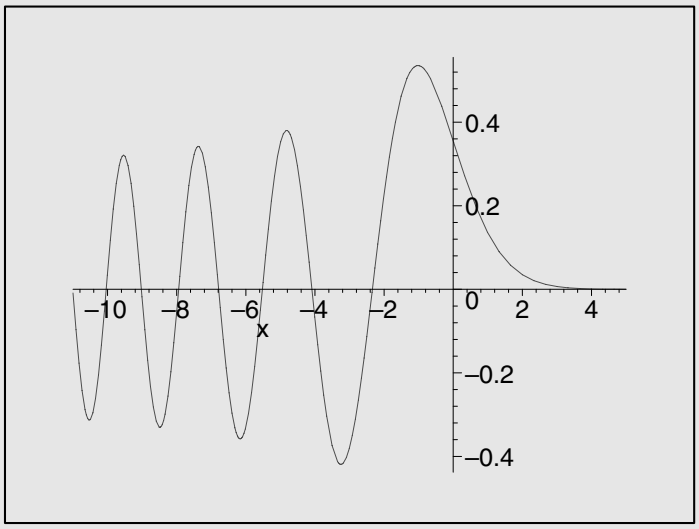
$$Eq1 := -\frac{1}{2}\frac{h_^2\left(\frac{d^2}{dx^2}\psi(x)\right)}{m} - F\,x\,\psi(x) = En\,\psi(x)$$

```
> Soln1 := dsolve(Eq1, psi(x));
```

$$Soln1 := \psi(x) = _C1\ \mathrm{AiryAi}\left(-\frac{2^{(1/3)}\left(\frac{F\,m}{h_^2}\right)^{(1/3)}(x\,F + En)}{F}\right) + _C2\ \mathrm{AiryBi}\left(-\frac{2^{(1/3)}\left(\frac{F\,m}{h_^2}\right)^{(1/3)}(x\,F + En)}{F}\right)$$

```
> plot(AiryAi(x), x=-11..5);
```

[2] See also J. J. Sakurai, *Modern Quantum Mechanics*, Reading, MA: Addison-Wesley, 1994, p. 107ff, in which the quantization condition can be approximately obtained using the old quantum theory due to Sommerfeld and Wilson.



With the definition of a dimensionless variable

$$\xi = \left(x + \frac{E}{F}\right)\left(\frac{2mF}{\hbar^2}\right)^{1/3}, \tag{15.41}$$

identified from the Maple output, one can verify that equation (15.40) (for $x < 0$) becomes

$$\frac{d^2\psi}{d\xi} + \xi\psi = 0, \tag{15.42}$$

which is the differential equation satisfied by an Airy function. We thus write the solution of the Schrödinger equation as

$$\psi(\xi) = \Phi(-\xi), \tag{15.43}$$

where $\Phi(\xi)$ denotes the Airy function.

From the definition of the dimensionless variable

$$\xi = \left(x + \frac{E}{F}\right)\left(\frac{2mF}{\hbar^2}\right)^{1/3},$$

and

$$\psi(x) = \Phi(-\xi),$$

the solution for $x < 0$ involves shifting the origin to the right by E/F, then inverting the Airy function with respect to the y axis. The symmetric nature of the potential energy requires $\psi(x)$ to be either even, for which $\psi(-x) = \psi(x)$, or odd, for which $\psi(-x) = -\psi(x)$. We discuss symmetric and antisymmetric solutions respectively. First, let

$$\tilde{E} = \frac{E}{\left(\frac{\hbar^2F^2}{2m}\right)^{1/3}}. \tag{15.44}$$

1. Symmetric function
   For a symmetric solution, because the wave function has an extremum at $x = 0$, the first derivative of the wave function must be zero at that point,

   $$\psi'(x = 0) = 0. \tag{15.45}$$

   We must have

   $$\psi'(x = 0) = \Phi'(-\tilde{E}) = 0. \tag{15.46}$$

   Discrete energies therefore correspond to the roots of the first derivative of the Airy function.

2. Antisymmetric function
   For an antisymmetric solution, because the wave function must pass the origin, we have

   $$\psi(x = 0) = 0, \tag{15.47}$$

   so

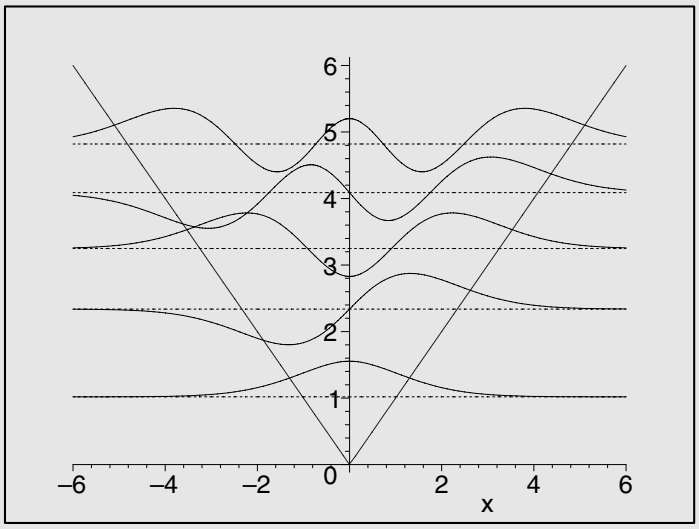
   $$\psi(x = 0) = \Phi(-\tilde{E}) = 0. \tag{15.48}$$

   Discrete energies correspond here to the roots of the Airy function.

Worksheet 15.6 In Maple, the Airy function is defined as `AiryAi(0,x)` and its derivative is defined as `AiryAi(1,x)` (the second argument indicates the 0th and 1st derivatives). We employ the `fsolve` command to find the roots numerically. The wave functions in the plot are not normalized.

```
> En0 := -fsolve(AiryAi(1,x)=0, x=-2..0);
                          En0 := 1.018792972
> En1 := -fsolve(AiryAi(x)=0, x=-3..-2);
                          En1 := 2.338107410
> En2 := -fsolve(AiryAi(1,x)=0, x=-4..-2);
                          En2 := 3.248197582
> En3 := -fsolve(AiryAi(x)=0, x=-5..-4);
                          En3 := 4.087949444
> En4 := -fsolve(AiryAi(1,x)=0, x=-6..-4);
                          En4 := 4.820099211
> p1:=plot([AiryAi(x-En0) + En0, En0, AiryAi(x-En1) + En1, En1,
> AiryAi(x-En2) + En2, En2, AiryAi(x-En3) + En3, En3,
> AiryAi(x-En4) + En4, En4, x], x=0..6):
```

```
> p2:=plot([AiryAi(-x-En0) + En0, En0, -AiryAi(-x-En1) + En1, En1,
> AiryAi(-x-En2) + En2, En2, -AiryAi(-x-En3) + En3, En3,
> AiryAi(-x-En4) + En4, En4, -x], x=-6..0):
> with(plots):
Warning, the name changecoords has been redefined
> display([p1, p2]);
```



Matching the Airy function to satisfy symmetry requirements, we obtain the wave functions and corresponding energies. We list the first five roots in Table 15.2, which are the values of discrete energies for this problem.

Table 15.2: Quantized energies in a homogeneous field.

n	$E/(F^2\hbar^2/2m)^{1/3}$
0	1.019
1	2.338
2	3.248
3	4.088
4	4.820

15.7 Morse Potential

The harmonic oscillator serves as a limiting model to approximate the potential energy of a stable diatomic molecule, but it is inadequate when two nuclei are far from their equilibrium separation. In 1929, P. M. Morse devised a potential-energy function that has a more realistic form,

$$V(x) = V_0(1 - e^{-\alpha x})^2, \tag{15.49}$$

where x measures the displacement from equilibrium. The Schrödinger equation for this potential reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (V_0 + V_0 e^{-2\alpha x} - 2V_0 e^{-\alpha x})\psi = E\psi; \tag{15.50}$$

as before, for bound states $E < V_0$. This problem is directly solvable with Maple. In this section, our intent is not to treat this problem in detail but to outline how a solution is obtained;[3] an additional discussion can be found in Appendix B.2.2.

In a similar way to the treatment of the harmonic oscillator, we introduce parameters to obtain a dimensionless equation that simplifies algebraic manipulation. From use of Maple to solve this Schrödinger equation directly, the result of which is listed in Appendix B.2.2, we define a dimensionless variable

$$\xi = \frac{2\sqrt{2mV_0}}{\alpha\hbar}e^{-\alpha x}; \tag{15.51}$$

we introduce two additional quantities,

$$s = \frac{\sqrt{2m(V_0 - E)}}{\alpha\hbar}, \quad n = \frac{2mV_0}{\alpha\hbar} - \left(s + \frac{1}{2}\right), \tag{15.52}$$

so as to simplify the Schrödinger equation, which becomes

$$\frac{d^2\psi}{d\xi^2} + \frac{1}{\xi}\frac{d\psi}{d\xi} + \left(-\frac{1}{4} + \frac{n + s + \frac{1}{2}}{\xi} - \frac{s^2}{\xi^2}\right)\psi = 0. \tag{15.53}$$

To solve this equation, we can again employ the method of series solution. We refrain from elaborating tedious mathematics, but simply state the result: the solution of equation (15.53) is

$$\psi_n = e^{\xi/2}\xi^s F(-n, 2s + 1; \xi), \tag{15.54}$$

where F is the confluent hypergeometric function, defined as

$$F(\alpha, \gamma; z) = 1 + \frac{\alpha}{\gamma}\frac{z}{1!} + \frac{\alpha(\alpha + 1)}{\gamma(\gamma + 1)}\frac{z^2}{2!} + \ldots. \tag{15.55}$$

[3]For more information, see L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, New York: Dover Publications, 1985, p. 271ff, or Landau and Lifshitz (*QM*) 1977, p. 72.

Having previously solved the Hermite equation directly, one should naturally appreciate that the solution of equation (15.53) can be expressed as a power series, which can be shown to be a confluent hypergeometric function.

Directly from the definition of the hypergeometric function, we deduce that only when α is zero or a negative integer can the series terminate at one particular term; hence $F(\alpha, \gamma; z)$ reduces to a polynomial of degree $|\alpha|$ in z. So for the wave function to remain finite, n must be a non-negative integer, and we again conclude that the energy must be quantized:

$$E_n = \hbar\sqrt{\frac{2V_0\alpha^2}{m}}\left(n+\frac{1}{2}\right) - \frac{\alpha^2\hbar^2}{2m}\left(n+\frac{1}{2}\right)^2, \tag{15.56}$$

for $E < V_0$.

In summary, the problem of the Morse potential has exact solutions; the discrete energies conform to equation (15.56), in which appears a residual energy for $n = 0$ as for the linear harmonic oscillator; the corresponding wave functions appear in equation (15.54).

We customarily normalize a wave function, so that the integral over all space of its associated probability density, which is the square of the wave function, is unity. The wave functions in equation (15.54) are not normalized, but we readily remedy this deficiency on evaluating

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2\, dx,$$

then dividing $\psi_n(x)$ by the square root of this integral.

Worksheet 15.7 The confluent hypergeometric function is defined as `hypergeom` in Maple. The normalized wave function is produced on dividing the unnormalized function by the square root of the integral of probability density over the entire region; such an integral is directly evaluated with Maple. The symbol `h` signifies $\hbar$, which is set to unity for graphic purpose.

```
> V0 := 20; alpha := 1; m := 1:  h := 1:
```

$$V0 := 20$$

$$\alpha := 1$$

```
> PE := V0*(1 - exp(-alpha*x))^2;
```

$$PE := 20\,(1 - e^{(-x)})^2$$

```
> xi := 2*sqrt(2*V0*alpha)/(alpha*h)*exp(-alpha*x);
```

$$\xi := 4\sqrt{10}\,e^{(-x)}$$

```
> En := h*sqrt(2*V0*alpha^2/m)*(n + 1/2) - alpha^2*h^2/(2*m)*(n +
> 1/2)^2; s := sqrt(2*(V0-En))/alpha;
```

$$En := 2\sqrt{10}\left(n+\frac{1}{2}\right) - \frac{\left(n+\frac{1}{2}\right)^2}{2}$$

$$s := \sqrt{40 - 4\sqrt{10}\left(n + \frac{1}{2}\right) + \left(n + \frac{1}{2}\right)^2}$$

```
> f := exp(-xi/2)*xi^(s)*hypergeom([-n], [2*s+1], xi);
```

$$f := e^{(-2\sqrt{10}\,e^{(-x)})}\,(4\sqrt{10}\,e^{(-x)})^{(\sqrt{40-4\sqrt{10}\,(n+1/2)+(n+1/2)^2})}$$

$$\text{hypergeom}\left([-n],\ \left[2\sqrt{40 - 4\sqrt{10}\,(n+\frac{1}{2}) + (n+\frac{1}{2})^2} + 1\right],\ 4\sqrt{10}\,e^{(-x)}\right)$$

```
> En0 := eval(En, n=0); f0 := eval(f, n=0);
```

$$En0 := \sqrt{10} - \frac{1}{8}$$

$$f0 := e^{(-2\sqrt{10}\,e^{(-x)})}\,(4\sqrt{10}\,e^{(-x)})^{(\sqrt{161/4-2\sqrt{10}})}$$

```
> En1 := eval(En, n=1); f1 := eval(f, n=1);
```

$$En1 := 3\sqrt{10} - \frac{9}{8}$$

$$f1 := e^{(-2\sqrt{10}\,e^{(-x)})}\,(4\sqrt{10}\,e^{(-x)})^{(\sqrt{169/4-6\sqrt{10}})}$$

$$\text{hypergeom}\left([-1],\ \left[2\sqrt{\frac{169}{4} - 6\sqrt{10}} + 1\right],\ 4\sqrt{10}\,e^{(-x)}\right)$$

```
> En2 := eval(En, n=2); f2 := eval(f, n=2);
```

$$En2 := 5\sqrt{10} - \frac{25}{8}$$

$$f2 := e^{(-2\sqrt{10}\,e^{(-x)})}\,(4\sqrt{10}\,e^{(-x)})^{(\sqrt{185/4-10\sqrt{10}})}$$

$$\text{hypergeom}\left([-2],\ \left[2\sqrt{\frac{185}{4} - 10\sqrt{10}} + 1\right],\ 4\sqrt{10}\,e^{(-x)}\right)$$

```
> En3 := eval(En, n=3); f3 := eval(f, n=3);
```

$$En3 := 7\sqrt{10} - \frac{49}{8}$$

$$f3 := e^{(-2\sqrt{10}\,e^{(-x)})}\,(4\sqrt{10}\,e^{(-x)})^{(\sqrt{209/4-14\sqrt{10}})}$$

$$\text{hypergeom}\left([-3],\ \left[2\sqrt{\frac{209}{4} - 14\sqrt{10}} + 1\right],\ 4\sqrt{10}\,e^{(-x)}\right)$$

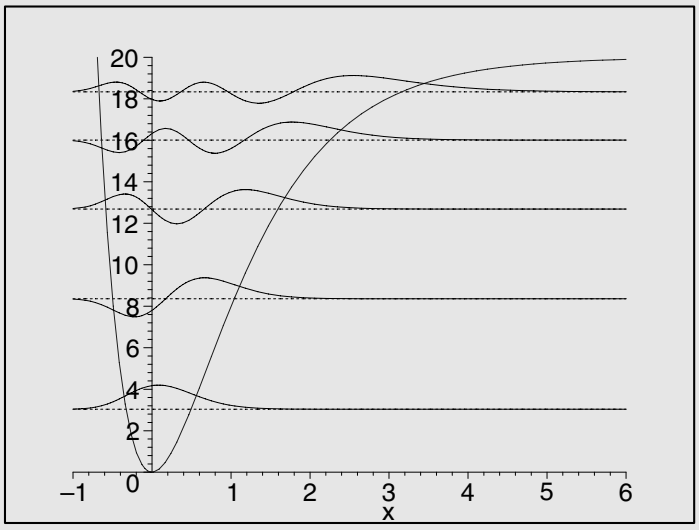
```
> En4 := eval(En, n=4); f4 := eval(f, n=4);
```

$$En4 := 9\sqrt{10} - \frac{81}{8}$$

$$f4 := e^{(-2\sqrt{10}\,e^{(-x)})}\,(4\sqrt{10}\,e^{(-x)})^{(\sqrt{241/4-18\sqrt{10}})}$$

$$\text{hypergeom}\left([-4],\left[2\sqrt{\frac{241}{4}-18\sqrt{10}}+1\right],\,4\sqrt{10}\,e^{(-x)}\right)$$

```
> F0 := f0/sqrt(evalf(int(f0^2, x=-infinity..infinity))):
> F1 := f1/sqrt(evalf(int(f1^2, x=-infinity..infinity))):
> F2 := f2/sqrt(evalf(int(f2^2, x=-infinity..infinity))):
> F3 := f3/sqrt(evalf(int(f3^2, x=-infinity..infinity))):
> F4 := f4/sqrt(evalf(int(f4^2, x=-infinity..infinity))):
> plot([En0, En0+F0, En1, En1+F1, En2, En2+F2, En3, En3+F3, En4,
> En4+F4, PE], x=-1..6, 0..V0, thickness=2);
```



The plot shows that the difference between two adjacent discrete energies is not constant, as for the harmonic oscillator, but decreases as n increases. Morse's analytic solution thus reproduces two properties of the vibrational spectra: (1) there are a finite number of discrete vibrational levels below V_0, and (2) the energy levels are more closely spaced with increasing n.

15.8 Bound Nonstationary States

So far, we have studied stationary states for bound states, each of which is a state with a definite energy. According to the principle of superposition, a linear combination of two wave functions also represents a possible quantum state. We use the wave functions for the harmonic oscillator to construct a nonstationary state as an example.

The complete wave function for a harmonic oscillator in its ground state is

$$\Psi_0(x,t) = \psi_0(x)e^{-iE_0t/\hbar} = e^{-\xi^2/2}e^{-i\omega t/2}, \tag{15.57}$$

and for the first excited state is

$$\Psi_1(x,t) = \psi_1(x)e^{-iE_1t/\hbar} = \sqrt{2}e^{-\xi^2/2}\xi e^{-3i\omega t/2}. \tag{15.58}$$

By adding the above two wave functions, we construct a state

$$\Psi(x,t) = \frac{1}{\sqrt{2}}[\Psi_0(x,t) + \Psi_1(x,t)], \tag{15.59}$$

which has an associated probability density

$$P(x,t) = \Psi^*(x,t)\Psi(x,t) = e^{-\xi^2/2}\left[\frac{1}{2} + \sqrt{2}\xi\cos(\omega t) + \xi^2\right]. \tag{15.60}$$

The mixed wave function $\Psi(x,t)$ is not a stationary state, because the probability density depends on time. This combined state oscillates at frequency ω. We leave it to an exercise to show that $\Psi(x,t)$ is not an eigenfunction of the Hamiltonian operator, hence that $\Psi(x,t)$ lacks a definite energy.

Worksheet 15.8 We produce an animation to demonstrate how the probability density from equation (15.60) depends on time.

```
> psi := (n,xi) ->
> (2^n*factorial(n))^(-1/2)*exp(-xi^2/2)*HermiteH(n,xi);
```

$$\psi := (n,\,\xi) \to \frac{e^{(-1/2\,\xi^2)}\,\mathrm{HermiteH}(n,\,\xi)}{\sqrt{2^n\,n!}}$$

```
> Psi0t := psi(0,xi)*exp(-I*t/2);
```

$$Psi0t := e^{(-\frac{\xi^2}{2})}\,\mathrm{HermiteH}(0,\,\xi)\,e^{(-1/2\,I\,t)}$$

```
> Psi1t := expand(psi(1,xi)*exp(-I*3*t/2));
```

$$Psi1t := \sqrt{2}\,e^{(-\frac{\xi^2}{2})}\,e^{(-3/2\,I\,t)}\,\xi$$

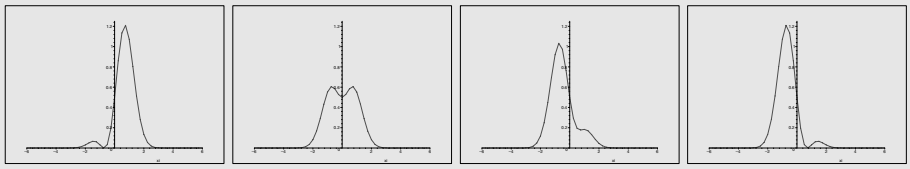
```
> Psimixed := 1/sqrt(2)*(Psi0t + Psi1t);
```

$$Psimixed := \frac{1}{2}\sqrt{2}\,(e^{(-\frac{\xi^2}{2})}\,\mathrm{HermiteH}(0,\,\xi)\,e^{(-1/2\,I\,t)} + \sqrt{2}\,e^{(-\frac{\xi^2}{2})}\,e^{(-3/2\,I\,t)}\,\xi)$$

```
> Epr1 := conjugate(Psimixed)*Psimixed:
> Epr2 := evalc(Epr1):
> Epr3 := combine(Epr2);
```

$$Epr3 := \frac{1}{2}\, e^{(-\xi^2)}\, \mathrm{HermiteH}(0,\, \xi)^2 + e^{(-\xi^2)}\, \mathrm{HermiteH}(0,\, \xi)\, \sqrt{2}\, \xi \cos(t) + e^{(-\xi^2)}\, \xi^2$$

```
> with(plots):
Warning, the name changecoords has been redefined
> animate(Epr3, xi=-6..6, t=0..2*Pi);
```



An energy eigenstate $\Psi_n(x,t)$ of a quantum-mechanical harmonic oscillator does not describe the familiar behavior of a classical oscillator: in the former case, the expectation value of x is stationary, instead of oscillating. From the above example, we see that a superposition of energy eigenstates might mimic oscillating behavior. By seeking a wave packet to bounce back and forth without spreading in shape, Schrödinger constructed a coherent state in 1926, which was a superposition of energy eigenstates,

$$\Psi_{(\lambda)}(x,t) = \sum_{n=0}^{\infty} f(n)\Psi_n(x,t), \tag{15.61}$$

where $|f(n)|^2$ is the Poisson distribution about the mean value μ,

$$|f(n)|^2 = \left(\frac{\mu^n}{n!}\right) e^{-\mu}. \tag{15.62}$$

We leave it as an exercise for the reader to construct a coherent state.

15.9 Two-state System

A two-state system of distinct energies is both the most fundamental and the most profound problem in quantum mechanics; it serves not only pedagogic but also practical purposes, such as to pertain to a maser or laser, magnetic resonance, neutrino oscillation, etc., to name just a few applications. In this section, we solve the problem of a symmetric potential with two

wells partitioned by a barrier, described by this function:

$$V(x) = \begin{cases} \infty, & x < -a - b/2, \\ 0, & -a - b/2 < x < -b/2, \\ V_0, & -b/2 < x < b/2, \\ 0, & b/2 < a + b/2, \\ \infty, & a + b/2 < x. \end{cases} \tag{15.63}$$

We take the states corresponding to the two least energies as an example of a two-state system.[4]

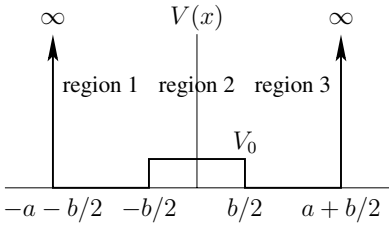


Figure 15.2: Double-well potential.

Similar to what we have routinely employed for a piecewise-constant potential, we denote regions with $-a - b/2 < x < b/2$, $-b/2 < x < b/2$ and $b/2 < x < a + b/2$ as 1, 2 and 3, respectively. The wave functions are

$$\begin{cases} \psi_1(x) = A \sin(k_1[x + a + b/2]), & -a - b/2 < x < -b/2, \\ \psi_2(x) = B_1 \sinh(\kappa_2 x) + B_2 \cosh(-\kappa_2 x), & -b/2 < x < b/2, \\ \psi_3(x) = C \sin(k_1[a + b/2 - x]), & b/2 < x < a + b/2. \end{cases} \tag{15.64}$$

Writing wave function $\psi_1(x)$ in this form, we have already taken into account a requirement that $\psi_1(-a - b/2)$ must be zero, with the same argument for $\psi_3(x)$. Instead of writing $e^{\pm\kappa_2 x}$, we express $\psi_2(x)$ in terms of $\sinh(\kappa_2 x)$ and $\cosh(\kappa_2 x)$, for subsequent convenience in relation to the symmetry property. As for many differential equations that we have already encountered, experience enables one to write general solutions in a form which will minimize rearrangement at a subsequent stage.

We have already employed boundary conditions at $x = -a - b/2$ and $x = a + b/2$; we impose four further continuity conditions:

$$\psi_1(-b/2) = \psi_2(-b/2), \tag{15.65a}$$

$$\psi_1'(-b/2) = \psi_2'(-b/2), \tag{15.65b}$$

$$\psi_2(b/2) = \psi_3(b/2), \tag{15.65c}$$

$$\psi_2'(b/2) = \psi_3'(b/2). \tag{15.65d}$$

[4] See also a discussion of the symmetrical double-well potential in J. J. Sakurai, *Modern Quantum Mechanics*, Reading, MA: Addison-Wesley, 1994, p. 256ff.

As this algebraic rearrangement resembles that in Section 15.3, we do not list the intermediate steps. For this symmetric potential, we again find two classes of solutions.

1. Symmetric function
   For a symmetric wave function, as we must have $B_1 = 0$, we reject the $\sinh(\kappa_2 x)$ term, and we have $C = A$. We obtain thereby the constraint for the energy,

$$\cot(k_1 a) = -\frac{\kappa_2}{k_1}\tanh(\kappa_2 b/2). \tag{15.66}$$

2. Antisymmetric function
   For an antisymmetric wave function, we must have $B_2 = 0$; we hence reject the $\cosh(\kappa_2 x)$ term, and we have $C = A$. We obtain another constraint for energy,

$$\tan(k_1 a) = -\frac{k_1}{\kappa_2}\tanh(\kappa_2 b/2). \tag{15.67}$$

We present a numerical example to further advance our discussion.

Example 15.2 A proton is subject to this symmetric double-well potential, for which $a = b = 0.5 \times 10^{-10}$ m, and $V_0 = 1.6 \times 10^{-19}$ J. Find the energies of the two lowest states and the corresponding wave functions.

Solution The energy levels can be found from the transcendental equations above. Applying the graphical and numerical method, we find the lowest values of the energy to be

$$E_{s1} = 1.102518 \times 10^{-20}\ \text{J}, \quad \text{(symmetric)},$$
$$E_{a1} = 1.102536 \times 10^{-20}\ \text{J}, \quad \text{(antisymmetric)}.$$

Once the energy is determined, we can solve for undetermined coefficients.

Worksheet 15.9 This worksheet is similar to that in Section 15.3. We produce an animation for each region 1, 2 and 3, and combine them in one plot using the `display` command. The symbol `h` stands for $\hbar$.

```
> psi1 := x -> A*sin(k1*(x + a + b/2));
```

$$\psi 1 := x \to A\sin\left(k1\ \left(x + a + \frac{b}{2}\right)\right)$$

```
> psi2 := x -> B1*sinh(kappa2*x) + B2*cosh(-kappa2*x);
```

$$\psi 2 := x \to B1\sinh(\kappa 2\, x) + B2\cosh(-\kappa 2\, x)$$

```
> psi3 := x -> C*sin(k1*(a + b/2 - x));
```

$$\psi 3 := x \to C\sin\left(k1\ \left(a + \frac{b}{2} - x\right)\right)$$

```
> Eq1 := psi1(-b/2) = psi2(-b/2);
```

$$Eq1 := A\sin(k1\ a) = -B1\sinh\left(\frac{\kappa 2\, b}{2}\right) + B2\cosh\left(\frac{\kappa 2\, b}{2}\right)$$

```
> Eq2 := D(psi1)(-b/2) = D(psi2)(-b/2);
```

$$Eq2 := A\cos(k1\ a)\, k1 = B1\cosh\left(\frac{\kappa 2\, b}{2}\right)\kappa 2 - B2\sinh\left(\frac{\kappa 2\, b}{2}\right)\kappa 2$$

```
> Eq3 := psi2(b/2) = psi3(b/2);
```

$$Eq3 := B1\sinh\left(\frac{\kappa 2\, b}{2}\right) + B2\cosh\left(\frac{\kappa 2\, b}{2}\right) = C\sin(k1\ a)$$

```
> Eq4 := D(psi2)(b/2) = D(psi3)(b/2);
```

$$Eq4 := B1\cosh\left(\frac{\kappa 2\, b}{2}\right)\kappa 2 + B2\sinh\left(\frac{\kappa 2\, b}{2}\right)\kappa 2 = -C\cos(k1\ a)\, k1$$

```
> B1 :=0; C := A;
```

$$B1 := 0$$
$$C := A$$

```
> Eq1; Eq2; Eq3; Eq4;
```

$$A\sin(k1\ a) = B2\cosh\left(\frac{\kappa 2\, b}{2}\right)$$

$$A\cos(k1\ a)\, k1 = -B2\sinh\left(\frac{\kappa 2\, b}{2}\right)\kappa 2$$

$$B2\cosh\left(\frac{\kappa 2\, b}{2}\right) = A\sin(k1\ a)$$

$$B2\sinh\left(\frac{\kappa 2\, b}{2}\right)\kappa 2 = -A\cos(k1\ a)\, k1$$

```
> Eq11 := isolate(Eq1, sin(k1*a));
```

$$Eq11 := \sin(k1\ a) = \frac{B2\cosh\left(\frac{\kappa 2\, b}{2}\right)}{A}$$

```
> Eq12 := isolate(Eq2, cos(k1*a));
```

$$Eq12 := \cos(k1\ a) = -\frac{B2\sinh\left(\frac{\kappa 2\, b}{2}\right)\kappa 2}{A\, k1}$$

```
> Eq13 := lhs(Eq12)/lhs(Eq11) = rhs(Eq12)/rhs(Eq11);
```

$$Eq13 := \frac{\cos(k1\ a)}{\sin(k1\ a)} = -\frac{\sinh\left(\frac{\kappa 2\, b}{2}\right)\kappa 2}{k1\cosh(\frac{\kappa 2\, b}{2})}$$

```
> A := 'A': B1 := 'B1':  B2 := 'B2':  C := 'C':
```

```
> B2 := 0; C := -A;
```

$$B2 := 0$$
$$C := -A$$

```
> Eq1; Eq2; Eq3; Eq4;
```

$$A\sin(k1\,a) = -B1\sinh\left(\frac{\kappa2\,b}{2}\right)$$

$$A\cos(k1\,a)\,k1 = B1\cosh\left(\frac{\kappa2\,b}{2}\right)\kappa2$$

$$B1\sinh\left(\frac{\kappa2\,b}{2}\right) = -A\sin(k1\,a)$$

$$B1\cosh\left(\frac{\kappa2\,b}{2}\right)\kappa2 = A\cos(k1\,a)\,k1$$

```
> Eq21 := isolate(Eq1, sin(k1*a));
```

$$Eq21 := \sin(k1\,a) = -\frac{B1\sinh\left(\frac{\kappa2\,b}{2}\right)}{A}$$

```
> Eq22 := isolate(Eq2, cos(k1*a));
```

$$Eq22 := \cos(k1\,a) = \frac{B1\cosh\left(\frac{\kappa2\,b}{2}\right)\kappa2}{A\,k1}$$

```
> Eq23 := lhs(Eq21)/lhs(Eq22) = rhs(Eq21)/rhs(Eq22);
```

$$Eq23 := \frac{\sin(k1\,a)}{\cos(k1\,a)} = -\frac{\sinh\left(\frac{\kappa2\,b}{2}\right)k1}{\cosh\left(\frac{\kappa2\,b}{2}\right)\kappa2}$$

```
> with(plots):
Warning, the name changecoords has been redefined
> m := 1.67e-27; h := 1.055e-34;
```

$$m := 0.167\,10^{-26}$$
$$h := 0.1055\,10^{-33}$$

```
> V0 := 1.6e-19; a := 0.5e-10; b := 0.5e-10;
```

$$V0 := 0.16\,10^{-18}$$
$$a := 0.5\,10^{-10}$$
$$b := 0.5\,10^{-10}$$

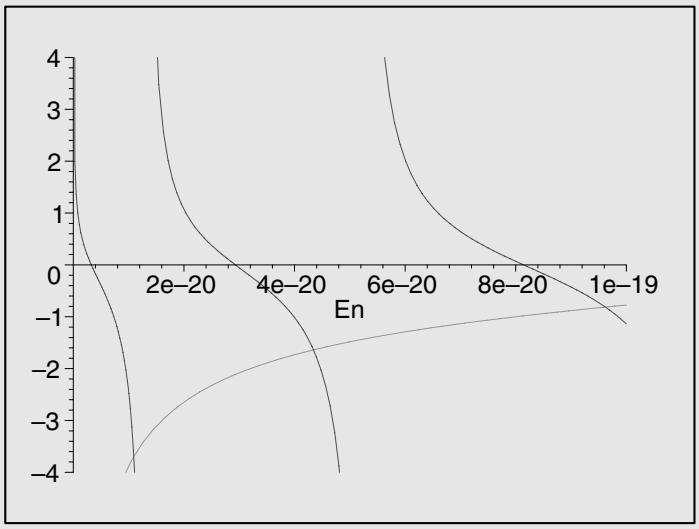
```
> br := piecewise(x>-b/2 and x<b/2, 1, x>-a, 0, x<a, 0):
> plbr := plot(br, x=-a-b/2..a+b/2, color=blue):
```

```
> k1 := sqrt(2*m*En)/h; kappa2 := sqrt(2*m*(V0-En))/h;
```

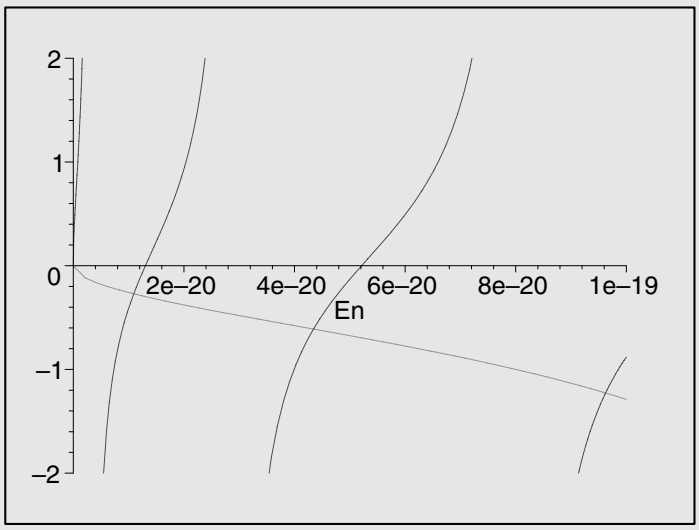
$$k1 := 0.5477984181\,10^{21}\sqrt{En}$$

$$\kappa 2 := 0.9478672986\,10^{34}\sqrt{0.5344\,10^{-45} - 0.334\,10^{-26}\,En}$$

```
> plot([lhs(Eq13), rhs(Eq13)], En=0..1e-19, -4..4, discont=true);
```




```
> plot([lhs(Eq23), rhs(Eq23)], En=0..1e-19, -2..2, discont=true);
```




```
> Es1 := fsolve(Eq13, En=1.5e-21..2e-20);
```

$$Es1 := 0.1102518089\,10^{-19}$$

```
> Ea1 := fsolve(Eq23, En=1.5e-21..2e-20);
```

$$Ea1 := 0.1102536279\,10^{-19}$$

```
> A := 'A': B1 := 'B1':  B2 := 'B2':  C := 'C': En := Es1;
```

$$En := 0.1102518089\,10^{-19}$$

```
> A := 1; B1 :=0; C := A;
```

$$A := 1$$
$$B1 := 0$$
$$C := 1$$

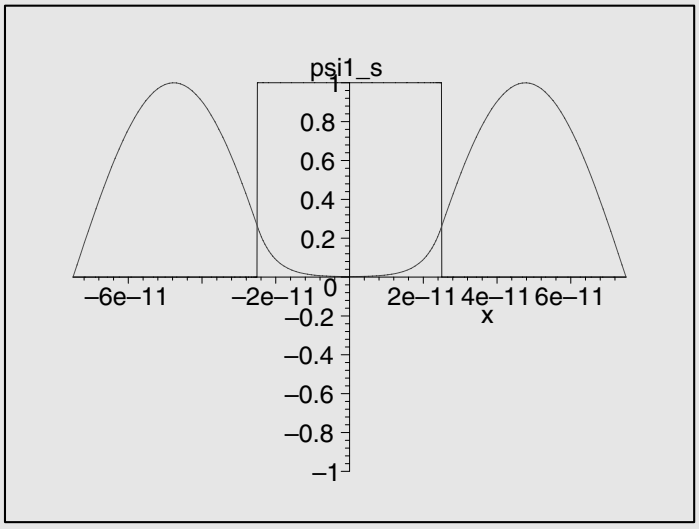
```
> Eq41 := Eq1;
```

$$Eq41 := 0.2625146824 = 98.76639633\,B2$$

```
> Eq42 := isolate(Eq41, B2);
```

$$Eq42 := B2 = 0.002657935210$$

```
> assign(Eq42);
> p1s1 := plot(psi1(x), x=-a-b/2..-b/2, -1..1):
> p2s1 := plot(psi2(x), x=-b/2..b/2):
> p3s1 := plot(psi3(x), x=b/2..a+b/2):
> Psi1s1 := psi1(x)*exp(-I*En/h*t):
> Psi2s1 := psi2(x)*exp(-I*En/h*t):
> Psi3s1 := psi3(x)*exp(-I*En/h*t):
> display([p1s1, p2s1, p3s1, plbr], title="psi1_s");
```




```
> A := 'A': B1 := 'B1':  B2 := 'B2':  C := 'C': En := Ea1;
```

$$En := 0.1102536279\,10^{-19}$$

```
> A := 1; B2 :=0; C := -A;
```

$$A := 1$$
$$B2 := 0$$
$$C := -1$$

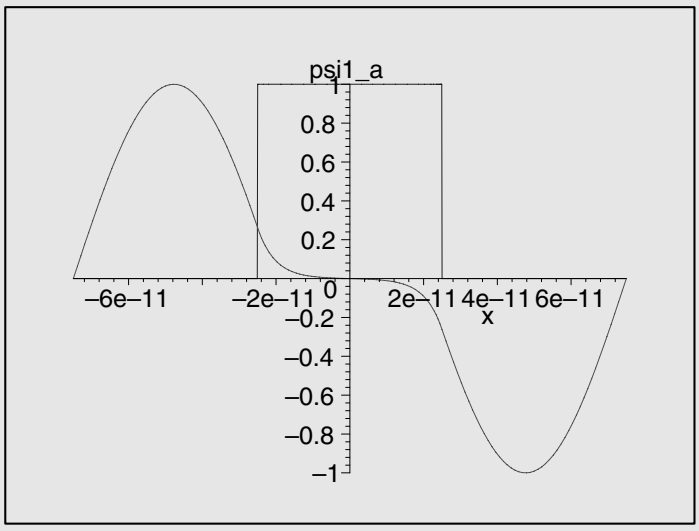
```
> Eq51 := Eq1;
```

$$Eq51 := 0.2624917884 = -98.76101474\,B1$$

```
> Eq52 := isolate(Eq51, B1);
```

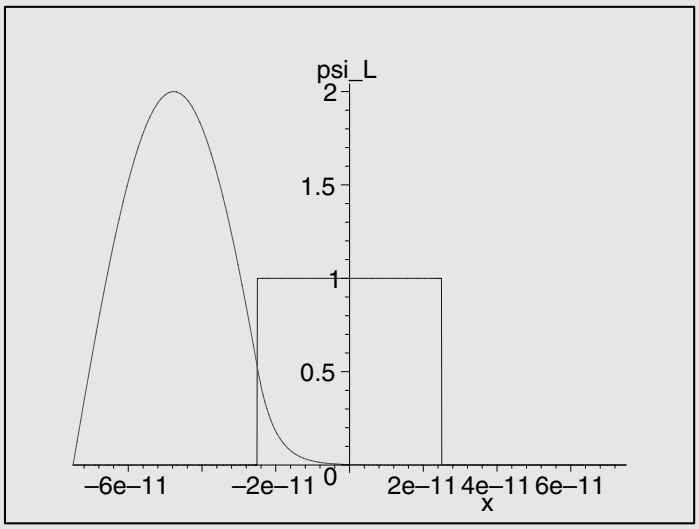
$$Eq52 := B1 = -0.002657848232$$

```
> assign(Eq52);
> p1a1 := plot(psi1(x), x=-a-b/2..-b/2, -1..1):
> p2a1 := plot(psi2(x), x=-b/2..b/2):
> p3a1 := plot(psi3(x), x=b/2..a+b/2):
> Psi1a1 := psi1(x)*exp(-I*En/h*t):
> Psi2a1 := psi2(x)*exp(-I*En/h*t):
> Psi3a1 := psi3(x)*exp(-I*En/h*t):
> display([p1a1, p2a1, p3a1, plbr], title="psi1_a");
```

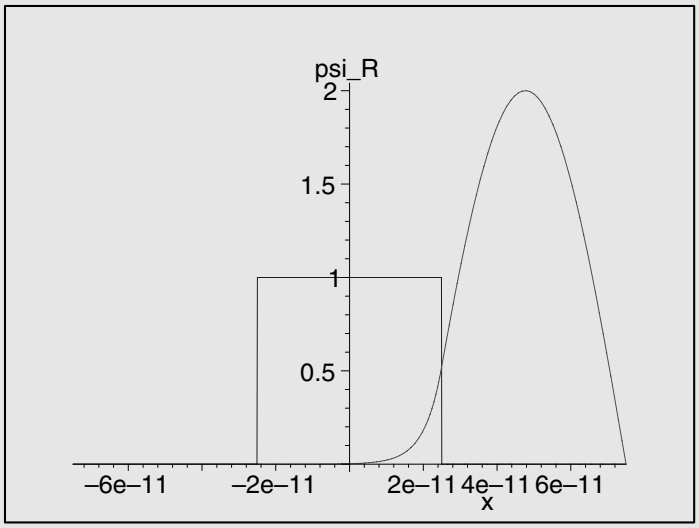



```
> Psi1l1 := Psi1s1 + Psi1a1:
> Psi2l1 := Psi2s1 + Psi2a1:
> Psi3l1 := Psi3s1 + Psi3a1:
> Psi1r1 := Psi1s1 - Psi1a1:
> Psi2r1 := Psi2s1 - Psi2a1:
> Psi3r1 := Psi3s1 - Psi3a1:
> panil1 := plot(Re(eval(Psi1l1, t=0)), x=-a-b/2..-b/2):
```

```
> panil2 := plot(Re(eval(Psi2l1, t=0)), x=-b/2..b/2):
> panil3 := plot(Re(eval(Psi3l1, t=0)), x=b/2..a+b/2):
> display([panil1, panil2, panil3, plbr], title="psi_L");
```




```
> panir1 := plot(Re(eval(Psi1r1, t=0)), x=-a-b/2..-b/2):
> panir2 := plot(Re(eval(Psi2r1, t=0)), x=-b/2..b/2):
> panir3 := plot(Re(eval(Psi3r1, t=0)), x=b/2..a+b/2):
> display([panir1, panir2, panir3, plbr], title="psi_R");
```



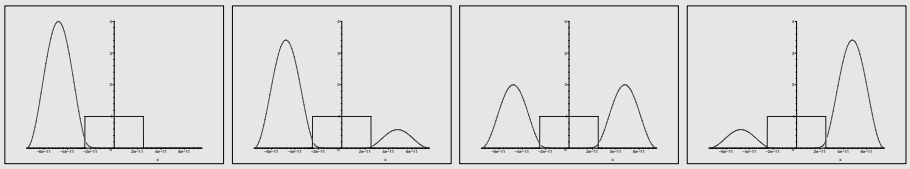
```
> T := 2*Pi/((Ea1 - Es1)/h);
```

$$T := 0.1159978010\,10^{-8}\,\pi$$

```
> pani1 := animate(Psi1l1*conjugate(Psi1l1), x=-a-b/2..-b/2,
t=0..T):

> pani2 := animate(Psi2l1*conjugate(Psi2l1), x=-b/2..b/2, t=0..T):

> pani3 := animate(Psi3l1*conjugate(Psi3l1), x=b/2..a+b/2, t=0..T):
> display([pani1, pani2, pani3, plbr]);
```



We denote the symmetric state of the least energy $\psi_{s1}(x)$, with energy E_{s1}, and the antisymmetric state of the least energy $\psi_{a1}(x)$, with energy E_{a1}. Our calculations show that

$$E_{a1} > E_{s1}, \tag{15.68}$$

which can be understood because the wave function of the antisymmetric state has a greater curvature. However, the energy difference is minute.

We form

$$\Psi_R(x,t) = \frac{1}{\sqrt{2}}\left(\psi_{s1}(x)e^{-iE_{s1}t/\hbar} + \psi_{a1}(x)e^{-iE_{a1}t/\hbar}\right), \tag{15.69}$$

and

$$\Psi_L(x,t) = \frac{1}{\sqrt{2}}\left(\psi_{s1}(x)e^{-iE_{s1}t/\hbar} - \psi_{a1}(x)e^{-iE_{a1}t/\hbar}\right). \tag{15.70}$$

The functions $\Psi_R(x,0)$ and $\Psi_L(x,0)$ are plotted above: the former concentrates on the right side of the double well, and the latter concentrates on the left. They are non-stationary states; the probability density $P_L(x,t)$ is

$$\begin{aligned}&\Psi_L^*(x,t)\Psi_L(x,t)\\ &\qquad = \frac{1}{2}\left\{\psi_{s1}^2(x) - 2\psi_{s1}(x)\psi_{a1}(x)\cos\left[\frac{(E_{a1}-E_{s1})t}{\hbar}\right] + \psi_{a1}^2(x)\right\}.\end{aligned} \tag{15.71}$$

Such a state oscillates at an angular frequency

$$\omega = \frac{E_{a1} - E_{s1}}{\hbar}, \tag{15.72}$$

so with period $T = 2\pi/\omega$. At $t = 0$, the probability density is

$$[\psi_{s1}(x) + \psi_{a1}(x)]^2 = [\Psi_L(x,0)]^2;$$

at $t = T/2$, the probability becomes

$$[\psi_{s1}(x) - \psi_{a1}(x)]^2 = [\Psi_R(x, 0)]^2,$$

which becomes concentrated on the right side. The animation shows how the system oscillates: it starts on the left side; after half a period it is found on the right side, then it returns to the left, and so forth.

This oscillation can be understood as a tunneling effect in quantum mechanics. A particle initially confined to the left side penetrates a finite barrier into the right side, then returns to the left side, and so on. As an application of this result, the ammonia molecule NH_3 can be crudely modeled with this potential, for which the vibrational barrier to inversion can be considered to be centered in a plane defined by three protons, with the N nucleus to the left or right. The frequency of oscillation for the ammonia molecule is about 24 GHz. With advanced quantum mechanics one can prove that application of an alternating electric field to this molecule can induce a resonance – a phenomenon similar to classical resonance; this property was utilized in constructing a maser and an atomic clock.

Exercises

1. Consider the potential energy for a finite well of the same form as in Section 15.3, except that $a = 1.8 \times 10^{-10}$ m and $V_0 = 120$ eV.

   (a) Find all possible energies for bound states.

   (b) Find the normalized wave function for energy states third and fourth from the minimum. For a symmetric solution for instance, express B_2 in terms of A, and $C = A$; in this way find A to normalize the wave function on solving the equation

   $$\int_{-\infty}^{-a/2} \psi_1^*(x)\psi_1(x)\,dx + \int_{-a/2}^{a/2} \psi_2^*(x)\psi_2(x)\,dx + \int_{a/2}^{\infty} \psi_3^*(x)\psi_3(x)\,dx = 1. \quad (15.73)$$

2. Consider solutions for the harmonic oscillator listed in Table 15.1.

   (a) Verify that ψ_0 and ψ_1 are eigenfunctions of the Hamiltonian operator for a harmonic oscillator, and find the eigenvalues.

   (b) Verify that

   $$\psi(x) = \frac{1}{\sqrt{2}}[\psi_0(x) + \psi_1(x)]$$

   is not an eigenfunction of the Hamiltonian operator, therefore that this state lacks a definite energy.

(c) The average energy for a nonstationary state is

$$\overline{E} = \frac{\int_{-\infty}^{\infty} \psi^*(x) H \psi(x)\, dx}{\int_{-\infty}^{\infty} \psi^*(x)\psi(x)\, dx}.$$

Evaluate this integral for the above combination of ψ_0 and ψ_1.

3. For solutions pertaining to a harmonic oscillator, evaluate the following integrals:

$$\int_{-\infty}^{\infty} \psi_1 x \psi_0\, dx, \quad \int_{-\infty}^{\infty} \psi_1 x \psi_1\, dx, \quad \int_{-\infty}^{\infty} \psi_1 x \psi_2\, dx.$$

Vary values of n relative to chosen fixed m and verify that

$$\int_{-\infty}^{\infty} \psi_n x \psi_m\, dx \neq 0 \quad \text{only if } m = n \pm 1. \tag{15.74}$$

This integral represents the matrix element of an electric dipole moment for a transition between initial state m and final state n. Application of this result to vibrational spectra of a diatomic molecule provides the explanation that most intense transitions occur between one state, labeled n, and an adjacent state, for which a selection rule is accordingly $\Delta n = \pm 1$.

4. For a particle of mass m subject to gravity, the one-dimensional potential is

$$V(x) = \begin{cases} mgx, & x > 0; \\ \infty, & x < 0. \end{cases} \tag{15.75}$$

The infinity can be considered as a hard surface.

(a) Evaluate the energy levels.

(b) Evaluate the expectation value $\overline{x^2}$ for the ground state.

Hint: the boundary condition requires that $\psi(x = 0) = 0$; consider existing solutions in Section 15.6.

5. The quantization rule of Bohr and Sommerfeld in the old quantum theory is

$$\frac{1}{2\pi\hbar} \oint p dx = n + \frac{1}{2}. \tag{15.76}$$

For the potential in equation (15.39), namely

$$V(x) = F|x|,$$

the quantization condition becomes

$$\frac{2}{2\pi\hbar} \int_{-E/F}^{E/F} \sqrt{2m(E - F|x|)}\, dx = n + \frac{1}{2} \tag{15.77}$$

because $p = \sqrt{2m(E-V)}$ and the classical turning points are $x = \pm E/F$. This integral is equivalent to

$$\frac{4}{2\pi\hbar}\int_0^{E/F}\sqrt{2m(E-Fx)}\,dx = n + \frac{1}{2}. \tag{15.77$'$}$$

Verify that

$$E_n = \frac{3^{2/3}}{4}(2\pi)^{2/3}\left(n+\frac{1}{2}\right)^{2/3}\left(\frac{F^2\hbar^2}{2m}\right)^{1/3}; \tag{15.78}$$

compare the results from this approximate method with the exact results in Table 15.2.

6. Construct a coherent state with (a) $\mu = 1$, (b) $\mu = 7$, according to equation (15.61). For $\mu = 1$, perform the summation from $n = 0$ to 5, and for $\mu = 7$, from $n = 0$ to 15. Animate the probability density, and observe the bouncing wave packet.

7. Unlike the potential energy for the harmonic oscillator, the Morse potential supports a finite number of discrete energy states; this fact is verifiable from equation (15.56). The number of bound states is one unit more than the value of n when E_n reaches a maximum for a bound state (because numbering with n begins at $n = 0$).

   (a) For the molecule $^1\mathrm{H}^{35}\mathrm{Cl}$, after the substitution of numerical values E_n (measured in joules) becomes

   $$E_n = 5.93\times10^{-20}\left(n+\frac{1}{2}\right) - 1.04\times10^{-21}\left(n+\frac{1}{2}\right)^2.$$

   Estimate the number of bound states for this system.

   (b) Derive a general formula for the quantum number for the most highly bound state in terms of V_0, α and m.

   Hint: for a maximum, the first derivative of E_n with respect to n is zero.

8. Find the next two energy levels for the double-well potential in Section 15.9. Are they close to each other? How can such a minute difference in energy be explained?

9. In an exercise in the preceding chapter, we briefly introduce the path integral formulation of quantum mechanics. This approach is inconvenient for practical problems in a nonrelativistic context: the calculation is difficult even for the simple harmonic oscillator, for which we only list the result:

$$\langle x,t|x_0,t_0\rangle = \tag{15.79}$$
$$\sqrt{\frac{m\omega}{2\pi i\hbar\sin[\omega(t-t_0)]}}\exp\left[\frac{im\omega}{2\hbar\sin[\omega(t-t_0)]}\left\{(x^2+x_0^2)\cos[\omega(t-t_0)]-2xx_0\right\}\right].$$

The reader should notice that the exponential part is $e^{iS/\hbar}$, where S is the classical action in equation (3.62). From this given result, show that $\langle x,t|x_0,t_0\rangle$ satisfies Schrödinger's time-dependent wave equation:

$$i\hbar\frac{\partial}{\partial t}\langle x,t|x_0,t_0\rangle = -\left(\frac{\hbar^2}{2m}\right)\frac{\partial^2}{\partial x^2}\langle x,t|x_0,t_0\rangle + \frac{m\omega^2x^2}{2}\langle x,t|x_0,t_0\rangle, \quad (15.80)$$

which serves as another example that the path integral is equivalent to wave mechanics.

10. The Lagrangian for a particle of mass m under the influence of gravity is

$$L = \frac{1}{2}m\dot{x}^2 - mgx; \quad (15.81)$$

the path integral for this system is

$$\langle x,t|x_0,t_0\rangle = \quad (15.82)$$
$$\sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\exp\left\{\frac{im}{\hbar}\left[\frac{(x-x_0)^2}{2(t-t_0)} - \frac{(t-t_0)}{2}g(x+x_0) - \frac{1}{24}g^2(t-t_0)^3\right]\right\};$$

the exponential of which one should compare with equation (3.60). Show that $\langle x,t|x_0,t_0\rangle$ satisfies Schrödinger's time-dependent wave equation:

$$i\hbar\frac{\partial}{\partial t}\langle x,t|x_0,t_0\rangle = -\left(\frac{\hbar^2}{2m}\right)\frac{\partial^2}{\partial x^2}\langle x,t|x_0,t_0\rangle + mgx\langle x,t|x_0,t_0\rangle, \quad (15.83)$$

which again demonstrates the link between path integral and wave mechanics.

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16 Schrödinger Equation in Three Dimensions

As a starting point, most textbooks on quantum mechanics rely on the Schrödinger equation. We have considered several fundamental and important topics concerning wave equations, such as problems on transmission and reflection involving a piecewise-constant potential in one dimension, time evolution of the Gaussian wave packet, a particle confined to a rigid well, a particle constrained to a rectangular well, the harmonic oscillator, the Morse oscillator, and so on. In this chapter, we discuss the Schrödinger equation in three dimensions in spherical coordinates. We solve equations for the Coulomb potential and for the infinite spherical well, which have practical applications in atomic and nuclear physics.

16.1 Central-force Problem

The generalization of differential operator $\partial^2/\partial x^2$ appearing in the one-dimensional Schrödinger equation to three dimensions is ∇^2, the Laplacian operator. The time-independent Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{16.1}$$

For a spherically symmetric potential $V(r)$, the use of spherical coordinates is convenient. In Section 7.5, we discovered how to express the Laplacian in spherical coordinates. The basic Schrödinger equation is thus explicitly written as

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi(r,\theta,\phi)}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi(r,\theta,\phi)}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi(r,\theta,\phi)}{\partial\phi^2}\right] + V(r)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi). \tag{16.2}$$

We use μ to denote the reduced mass in order to avoid confusion with m, which is the symbol for the magnetic quantum number later on.

As for many partial differential equations that we have already solved, we employ a product of functions to separate the variables,

$$\psi(r,\theta,\phi) = R(r)Y_{lm}(\theta,\phi), \tag{16.3}$$

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and thus obtain an angular equation,

$$-\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]Y_{lm}=l(l+1)Y_{lm}, \tag{16.4}$$

and a radial equation,

$$-\frac{\hbar^2}{2\mu r^2}\frac{d}{dr}\left[r^2\frac{dR(r)}{dr}\right]+\left[\frac{l(l+1)\hbar^2}{2\mu r^2}+V(r)\right]R(r)=ER(r), \tag{16.5}$$

where $l(l+1)$ is a constant of separation. Discussion of these two equations follows.

16.2 Spherical Harmonics

In Chapter 7, we stated that any function satisfying the Laplace equation is a harmonic function. In spherical coordinates, the angular part of the Schrödinger equation is none other than the angular part of the Laplace equation, and the solution is called spherical harmonics, with a symbol $Y_{lm}(\theta,\phi)$. In Chapter 7 we restricted ourselves to the situation in which there is azimuthal symmetry, namely $m=0$; here we remove such a restriction. Our discussion below is useful in both quantum mechanics and boundary-value problems in electrostatics.

We let $Y_{lm}=\Phi(\phi)\Theta(\theta)$, and substitute it into the angular equation,

$$\frac{-\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-l(l+1)\sin^2\theta=\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}, \tag{16.6}$$

so that dependences on θ and ϕ can be further separated; expressions on both sides of the equation must equal the same constant, taken to be $-m^2$:

$$\frac{d^2\Phi}{d\phi^2}=-m^2\Phi, \tag{16.7}$$

and

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-\left[l(l+1)-\frac{m^2}{\sin^2\theta}\right]\Theta=0. \tag{16.8}$$

The azimuthal equation is easy to solve:

$$\Phi(\phi)=e^{\pm im\phi}. \tag{16.9}$$

For $\Phi(\phi)$ to be single-valued, m must be an integer, accordingly known as the azimuthal or magnetic quantum number.

We make a change of variable by letting $\cos\theta=x$ so that $\Theta(\theta)=P(x)$; the equation for θ becomes

$$(1-x^2)\frac{d^2P(x)}{dx^2}-2x\frac{dP(x)}{dx}+\left[l(l+1)-\frac{m^2}{1-x^2}\right]P(x)=0. \tag{16.10}$$

This equation is called the generalized Legendre equation; its solutions are the associated Legendre functions. The approach used to solve this differential equation is similar to what we have done before: we can use a series expansion as illustrated in Section 15.4 (Hermite equation) and Appendix B.1. The essential idea is that, for this infinite series to terminate at a particular term, l must be 0 or a positive integer. Without proof we state that, for the generalized Legendre equation, the allowed range of m is from $-l$ to $+l$; one can verify this statement by obtaining the recurrence relation for this equation. The associated Legendre functions $P_{lm}(x)$ are well studied, and are defined in Maple. When using special functions, one must devote attention to their definitions because they are not universally agreed in the literature. Instead of calling `LegendreP` in Maple, we can directly generate the associated Legendre polynomials using Rodrigues' formula:

$$P_{lm}(x) = \frac{1}{2^l l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l \quad \text{for } m \geq 0. \tag{16.11}$$

The product of P and Φ is the solution of the angular part of the wave function. According to the above definition, we write the spherical harmonics

$$Y_{lm}(\theta,\phi), \quad l = 0,1,2,\ldots, \quad m = -l,-l+1,\ldots,+l, \tag{16.12}$$

as

$$\begin{cases} Y_{lm}(\theta,\phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_{lm}(\cos\theta)e^{im\phi} & \text{for } m \geq 0, \\ Y_{lm}(\theta,\phi) = (-1)^{|m|} Y^*_{l|m|}(\theta,\phi) & \text{for } m < 0. \end{cases} \tag{16.13}$$

Hence the angular part of the solution of the Schrödinger equation is the spherical harmonics $Y_{lm}(\theta,\phi)$. Spherical harmonics are normalized orthogonal functions:

$$\int_0^{2\pi} d\phi \int_{-1}^{+1} d(\cos\theta) Y^*_{l'm'}(\theta,\phi) Y_{lm}(\theta,\phi) = \delta_{ll'}\delta_{mm'}. \tag{16.14}$$

Worksheet 16.1 Instead of using `LegendreP` defined in Maple, we use Rodrigues' formula in equation (16.11), which involves multiple differentiations, to generate the associated Legendre polynomials. Spherical harmonics follow directly from equation (16.13).

```
> P := (l, m, x) ->
> 1/(2^l*l!)*(1-x^2)^(m/2)*diff((x^2-1)^l,x$(l+m));
```

$$P := (l,\, m,\, x) \to \frac{(1-x^2)^{(1/2\,m)}\,(\frac{d^{l+m}}{dx^{l+m}}\,(x^2-1)^l)}{2^l\,l!}$$

```
> Y := (l, m, theta, phi) ->
> (-1)^(m)*sqrt((2*l+1)/(4*Pi)*(l-m)!/(l+m)!)*subs(x=cos(theta),
> P(l,m,x))*exp(I*m*phi);
```

$$Y := (l,\, m,\, \theta,\, \phi) \to (-1)^m \sqrt{\frac{1}{4}\,\frac{(2\,l+1)\,(l-m)!}{\pi\,(l+m)!}}\,\mathrm{subs}(x=\cos(\theta),\, \mathrm{P}(l,\, m,\, x))\, e^{(m\,\phi\,I)}$$

```
> Y(1, 0, theta, phi);
```

$$\frac{1}{2}\,\frac{\sqrt{3}\cos(\theta)}{\sqrt{\pi}}$$

```
> Y(1, 1, theta, phi);
```

$$-\frac{1}{4}\,\frac{\sqrt{6}\,\sqrt{1-\cos(\theta)^2}\,e^{(\phi\,I)}}{\sqrt{\pi}}$$

```
> Y(2, 0, theta, phi);
```

$$\frac{1}{2}\,\frac{\sqrt{5}\,(\frac{3}{2}\cos(\theta)^2-\frac{1}{2})}{\sqrt{\pi}}$$

```
> Y(2, 1, theta, phi);
```

$$-\frac{1}{4}\,\frac{\sqrt{30}\,\sqrt{1-\cos(\theta)^2}\cos(\theta)\,e^{(\phi\,I)}}{\sqrt{\pi}}$$

```
> Y(2, 2, theta, phi);
```

$$\frac{1}{24}\,\frac{\sqrt{30}\,(3-3\cos(\theta)^2)\,e^{(2\,I\,\phi)}}{\sqrt{\pi}}$$

```
> Y(3, 0, theta, phi);
```

$$\frac{1}{2}\,\frac{\sqrt{7}\,(\cos(\theta)^3+\frac{3}{2}\,(\cos(\theta)^2-1)\cos(\theta))}{\sqrt{\pi}}$$

```
> Y(3, 1, theta, phi);
```

$$-\frac{1}{576}\,\frac{\sqrt{21}\,\sqrt{1-\cos(\theta)^2}\,(360\cos(\theta)^2-72)\,e^{(\phi\,I)}}{\sqrt{\pi}}$$

```
> Y(3, 2, theta, phi);
```

$$\frac{1}{8}\,\frac{\sqrt{210}\,(1-\cos(\theta)^2)\cos(\theta)\,e^{(2\,I\,\phi)}}{\sqrt{\pi}}$$

```
> Y(3, 3, theta, phi);
```

$$-\frac{1}{8}\,\frac{\sqrt{35}\,(1-\cos(\theta)^2)^{(3/2)}\,e^{(3\,I\,\phi)}}{\sqrt{\pi}}$$

We list spherical harmonics $Y_{lm}(\theta,\phi)$ for small values of l in Table 16.1; these functions are useful as a basis for expansion in spherical coordinates. An arbitrary function $g(\theta,\phi)$ can be expanded in spherical harmonics,

$$g(\theta,\phi)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}A_{lm}Y_{lm}(\theta,\phi), \tag{16.15a}$$

where the coefficients are

$$A_{lm}=\int_0^{2\pi}d\phi\int_{-1}^{+1}d(\cos\theta)Y_{lm}^*(\theta,\phi)g(\theta,\phi). \tag{16.15b}$$

Table 16.1: Spherical harmonics $Y_{lm}(\theta,\phi)$.

l	m	
	0	±1
0	$\frac{1}{\sqrt{4\pi}}$	0
1	$\sqrt{\frac{3}{4\pi}}\cos\theta$	$\mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}$
2	$\sqrt{\frac{5}{16\pi}}(3\cos^2\theta-1)$	$\mp\sqrt{\frac{15}{8\pi}}(\sin\theta\cos\theta)e^{\pm i\phi}$
3	$\sqrt{\frac{7}{16\pi}}(5\cos^3\theta-3\cos\theta)$	$\mp\sqrt{\frac{21}{64\pi}}(5\cos^2\theta-1)\sin\theta e^{\pm i\phi}$
l	m	
	±2	±3
0	0	0
1	0	0
2	$\sqrt{\frac{15}{32\pi}}(\sin^2\theta)e^{\pm2i\phi}$	0
3	$\sqrt{\frac{210}{64\pi}}\cos\theta\sin^2\theta e^{\pm2i\phi}$	$\mp\sqrt{\frac{35}{64\pi}}\sin^3\theta e^{\pm3i\phi}$

With these spherical harmonics, we are in a position to complete the treatment of electrostatics in spherical coordinates, first introduced in Section 6.4.2 and Section 7.5. In equation (7.47), we express a potential with azimuthal symmetry in terms of Legendre polynomials,

$$V(r,\theta)=\sum_{l=0}^{\infty}\left(A_l r^l+\frac{B_l}{r^{l+1}}\right)P_l(\cos\theta). \tag{16.16}$$

The solution of a boundary-value problem without azimuthal symmetry is naturally

$$V(r,\theta,\phi)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(A_{lm}r^l+\frac{B_{lm}}{r^{l+1}}\right)Y_{lm}(\theta,\phi). \tag{16.17}$$

Recall equation (6.47): for two position vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ with spherical coordinates (r_1, θ_1, ϕ_1) and (r_2, θ_2, ϕ_2), respectively (referring to Figure 6.5), we can expand $|\mathbf{r}_1 - \mathbf{r}_2|^{-1}$ as

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\gamma), \tag{16.18}$$

where $r_<$ ($r_>$) is the smaller (larger) of $|\mathbf{r}_1|$ and $|\mathbf{r}_2|$, and γ is the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$, which can be expressed as

$$\cos\gamma = \cos\theta_2 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2). \tag{16.19}$$

The addition theorem of spherical harmonics is

$$P_l(\cos\gamma) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}^*(\theta_2, \phi_2) Y_{lm}(\theta_1, \phi_1). \tag{16.20}$$

This result is simply an application of equation (16.15), which we omit in the proof of this theorem.[1] In sum, the most general expansion of $|\mathbf{r}_1 - \mathbf{r}_2|^{-1}$ in spherical coordinates is

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{1}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_{lm}^*(\theta_2, \phi_2) Y_{lm}(\theta_1, \phi_1). \tag{16.21}$$

This expansion is useful in many calculations; see Section 16.5.1.

16.3 Angular Momentum

The operator which represents the square of the total angular momentum in quantum mechanics is

$$L^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right], \tag{16.22}$$

which can be derived from the definition of the angular momentum; classically, $\mathbf{L} = \mathbf{r} \times \mathbf{p}$. If we make the conventional Schrödinger substitution, we find that

$$L_x = -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right), \quad L_y = -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right), \quad L_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right). \tag{16.23}$$

Transforming these relations to spherical coordinates, which requires tedious algebraic manipulation, we can verify the L^2 operator. The operator which represents the z component of angular momentum has a simple expression:

$$L_z = -i\hbar \frac{\partial}{\partial\phi}. \tag{16.24}$$

[1] See Jackson 1999, p. 110ff.

The square of the angular momentum operator L^2 is essentially the angular part of the Laplacian operator in spherical coordinates:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2}. \tag{16.25}$$

We already know the solutions of the angular part of the Laplacian operator, which are spherical harmonics.

Let us review what we have learned about wave mechanics. The time-dependent Schrödinger equation in three dimensions is

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t) = -\frac{\hbar}{i}\frac{\partial\Psi(\mathbf{r},t)}{\partial t}. \tag{16.26}$$

From Section 14.1, we know that, if the potential energy contains no explicit dependence on t, we can separate the Schrödinger equation into a spatial equation and a temporal equation. The constant of separation, E, is the energy, and the temporal part of the equation has a simple form, namely

$$f(t) = \exp\left(-\frac{iEt}{\hbar}\right). \tag{16.27}$$

We then focus on solving the time-independent Schrödinger equation. In this chapter, we find that, if the potential energy contains no explicit term depending on angles θ and ϕ, we can separate the time-independent Schrödinger equation into an angular equation and a radial equation. The constant of separation $l(l+1)$ is related to the angular momentum, and the solution of the angular part of the equation involves spherical harmonics $Y_{lm}(\theta,\phi)$. Recall that the temporal function $f(t)$ is an eigenfunction of the Hamiltonian operator,

$$Hf(t) = -\frac{\hbar}{i}\frac{\partial}{\partial t}f(t) = Ef(t), \tag{16.28}$$

for which the eigenvalue is E. Spherical harmonics are analogously eigenstates of the operator for the square of the angular momentum,

$$L^2 Y_{lm}(\theta,\phi) = l(l+1)\hbar^2 Y_{lm}(\theta,\phi), \tag{16.29}$$

and for a projection of angular momentum on one axis, commonly taken to be z,

$$L_z Y_{lm}(\theta,\phi) = m\hbar Y_{lm}(\theta,\phi). \tag{16.30}$$

The eigenvalue for the square of the angular momentum is $l(l+1)\hbar^2$, and for its projection on the z axis is $m\hbar$. We call l the quantum number of total angular momentum, and m the magnetic or azimuthal quantum number. Purely from mathematical properties of the Legendre equation, l must be 0 or a positive integer, and m must be an integer ranging from $-l$ to $+l$, so that the wave function remains single-valued and finite. The requirements for a wave function to satisfy the Schrödinger equation lead to quantization of angular momentum.

For any problem involving a central force, the solution of the angular part involves spherical harmonics; hence we only concentrate on the radial part, which is reduced to an equivalent one-dimensional problem – solving an ordinary differential equation.

16.4 Coulomb Potential

We discuss the Schrödinger equation under the Coulomb potential, which is the wave-mechanical treatment of the hydrogen atom. The radial equation for this potential is

$$-\frac{h^2}{8\pi^2\mu r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)+\left[\frac{l(l+1)h^2}{8\pi^2\mu r^2}-\frac{e^2}{4\pi\epsilon_0 r}\right]R(r)=ER(r). \tag{16.31}$$

Although this problem is well treated, with $R(r)$ related to the associated Laguerre polynomials, here we employ the method of power series, the same method in our discussion of the Hermite equation in Section 15.4, to obtain the solution from the beginning, so that we enhance our comprehension of the quantization of energy. Moreover, we will discover degeneracy, which is a property absent from the Schrödinger equation in one dimension. To tackle the differential equation, we first introduce dimensionless parameters to express the equation in a simplified form. We measure radius in terms of the Bohr radius a_0, and energy in terms of potential energy at the Bohr radius,[2]

$$r=a_0\rho=\frac{h^2\epsilon_0}{\pi\mu e^2}\rho,\quad E=-|E|=-\frac{\mu e^4}{4h^2\epsilon_0^2}\varepsilon. \tag{16.32}$$

With these transformed parameters, we obtain

$$\frac{d^2R(\rho)}{d\rho^2}+\frac{2}{\rho}\frac{dR(\rho)}{d\rho}+\left[-2\varepsilon+\frac{2}{\rho}-\frac{l(l+1)}{\rho^2}\right]R(\rho)=0. \tag{16.33}$$

We further simplify the equation on observing the asymptotic behavior. For large ρ, we have an approximate equation $R''=2\varepsilon R$, which has a solution $R=e^{-\sqrt{2\varepsilon}\rho}$. We let

$$R(\rho)=e^{-\sqrt{2\varepsilon}\rho}f(\rho), \tag{16.34}$$

so that the equation becomes

$$\frac{d^2f}{d\rho^2}+2\left(\frac{1}{\rho}-\sqrt{2\varepsilon}\right)\frac{df}{d\rho}+\left[\frac{2(1-\sqrt{2\varepsilon})}{\rho}-\frac{l(l+1)}{\rho^2}\right]f=0. \tag{16.35}$$

This equation has a singularity at $\rho=0$. To use a power series to represent the solution, we multiply the power series by ρ^q; then the solution takes a form

$$f=\rho^q\sum_{k=0}^{\infty}a_k\rho^k. \tag{16.36}$$

In developing the recurrence relation as before, we must determine q. Collecting coefficients of the ρ^q term, we obtain an indicial equation,

$$(q-l)(q+l+1)=0. \tag{16.37}$$

[2]The numerical value is twice the Rydberg energy: $\frac{e^2}{4\pi\epsilon_0 a_0}=4.359\times10^{-18}$ J $=27.21$ eV; it is commonly called the atomic unit of energy or *hartree*.

The root of this equation is $q = l$ or $q = -(l+1)$. Using $q = l$, we obtain a recurrence relation,

$$a_{k+1} = 2\frac{(k+l+1)\sqrt{2\varepsilon} - 1}{(k+1)(k+2l+2)}a_k. \tag{16.38}$$

To make the series finite, we must have it terminate at $k = n_r$, so that $a_{n_r+1} = a_{n_r+2} = \ldots = 0$; namely,

$$\sqrt{2\varepsilon} = \frac{1}{n_r + l + 1}. \tag{16.39}$$

We define n_r as the radial quantum number. Let $n = n_r + l + 1$; from the definition of ε, we have

$$E_n = -\frac{1}{n^2}\frac{\mu e^4}{8h^2\epsilon_0^2}, \tag{16.40}$$

which is the same result as Bohr's model for energies of stationary states. Quantization of energy is again a consequence of the requirement that a wave function must remain finite.

We call n the principal quantum number, because it determines the total energy of a quantum state. For a particular n, there are n possible values of l, that is $l = 0, 1, \ldots, n-1$; for each value of l, there are $2l+1$ possible values of m, that is $m = -l, -l+1, \ldots, l-1, l$. Quantum states described by distinct wave functions but associated with the same energy are said to be *degenerate*; degeneracy is a phenomenon that occurs only for dimensions more than one. As a simple exercise, one can verify that for each value of n, there are n^2 degenerate eigenfunctions in total.

Worksheet 16.2 The technique of deriving a recurrence relation using Maple is almost the same as in Section 15.4 and Appendix B.1, except here we first need to obtain the indicial equation and its roots. Choosing the root l, we return to the differential equation again; generally five consecutive terms are sufficient to derive the recurrence relation.

```
> f := sum(a[k]*rho^(k+q), k=0..5);
```

$$f := a_0\,\rho^q + a_1\,\rho^{(1+q)} + a_2\,\rho^{(2+q)} + a_3\,\rho^{(3+q)} + a_4\,\rho^{(4+q)} + a_5\,\rho^{(5+q)}$$

```
> Eq1 := diff(f, rho$2) + (2/rho - 2*sqrt(2*epsilon))*diff(f, rho)
> + (2/rho*(1-sqrt(2*epsilon)) - l*(l+1)/rho^2)*f = 0:
> Eq2 := simplify(Eq1):
> Eq3 := map(coeff, Eq2, rho^q):
> Eq4 := factor(Eq3);
```

$$Eq4 := -\frac{a_0\,(l+1+q)\,(l-q)}{\rho^2} = 0$$

```
> restart:
```

```
> f := sum(a[i]*rho^(i+l), i=k-2..k+2);
```

$$f := a_{k-2}\,\rho^{(-2+k+l)} + a_{-1+k}\,\rho^{(-1+k+l)} + a_k\,\rho^{(k+l)} + a_{1+k}\,\rho^{(1+k+l)} + a_{k+2}\,\rho^{(2+k+l)}$$

```
> Eq1 := diff(f, rho$2) + (2/rho - 2*sqrt(2*epsilon))*diff(f, rho)
> + (2/rho*(1-sqrt(2*epsilon)) - l*(l+1)/rho^2)*f = 0:
> Eq2 := simplify(Eq1):
> Eq3 := map(coeff, Eq2, rho^(k+1+l)):
> Eq4 := isolate(Eq3, a[k+1]):
> Eq5 := factor(Eq4);
```

$$Eq5 := a_{1+k} = \frac{2\,a_k\,(\sqrt{2}\,\sqrt{\varepsilon}\,l + \sqrt{2}\,\sqrt{\varepsilon}\,k - 1 + \sqrt{2}\,\sqrt{\varepsilon})}{(1+k)\,(k+2+2\,l)}$$

The solution of equation (16.35) is

$$f_1 = \rho^l \left(a_0 + a_1\rho + a_2\rho^2 + a_3\rho^3 + \ldots\right), \tag{16.41}$$

where a_k conforms to the recurrence relation. A second-order differential equation ought to have two independent solutions. From the indicial equation, one might think that the second solution can be obtained from the other root of the indicial equation, $q = -(l+1)$. However, if roots of the indicial equation differ by an integer, as in this case, the second solution from $q = -(l+1)$ is not independent of the first one from $q = l$. The second solution contains a logarithmic term, which has the form:[3]

$$f_2 = a f_1 \ln\rho + \rho^{-l-1}\left(\sum_{k=0}^{\infty} c_k \rho^k\right). \tag{16.42}$$

In the present example, f_2 is an unsuitable solution because it is not square integrable; we refrain from discussing it further. Many textbooks discard the root $-(l+1)$ of the indicial equation without mentioning this subtle property of differential equation.

16.5 Hydrogen Atom

In the preceding section, we derived the quantization of energy levels from solving the differential equation directly. To write the radial solution more compactly, we use the well established solutions for the Coulomb potential: the associated Laguerre polynomials. These polynomials are defined as

$$L_p^q(x) = \frac{d^q}{dx^q} L_p(x), \tag{16.43}$$

[3]The general theory is fairly complicated; see Boyce and DiPrima 2001, p. 277ff.

where L_p are Laguerre polynomials that can be generated by Rodrigues' formula:

$$L_p(x) = e^x \frac{d^p}{dx^p}(x^p e^{-x}). \tag{16.44}$$

We again caution the reader that the definitions of these special functions differ in detail among various sources.

According to the above definition, the radial part of the normalized wave function for the hydrogen atom is

$$R_{nl} = -\frac{1}{a_0^{3/2}} \frac{2}{n^2} \sqrt{\frac{(n-l-1)!}{[(n+l)!]^3}} e^{-\rho/n} \left(\frac{2\rho}{n}\right)^l L_{n+l}^{2l+1}\left(\frac{2\rho}{n}\right), \tag{16.45}$$

where ρ is the ratio of the radius to the Bohr radius, $\rho = r/a_0$, as defined in preceding section.[4]

Worksheet 16.3 Although Maple essentially defines all the special functions, one must be aware that the definition of these functions are not universally agreed among literature. For example, `LaguerreL` differs from equation (16.44) by a factor of $p!$. One should consult help to find the convention of `LaguerreL` in Maple; we create `altLaguerreL` to make it consistent with our discussion above. We use this worksheet to generate the radial part of the solutions of the hydrogen atom, as well as their plots. For graphical purposes, a_0 is set to unity.

```
> altLaguerreL := (n,a,x) -> (-1)^a*n!*LaguerreL(n-a,a,x):
> R := (n, l, r) -> -2/n^2*sqrt((n-l-1)!/((n+l)!)^3)*
> exp(-r/n)*(2*r/n)^l*altLaguerreL(n+l, 2*l+1, 2*r/n);
```

$$R := (n,\, l,\, r) \rightarrow -\frac{2\sqrt{\frac{(n-l-1)!}{((n+l)!)^3}}\, e^{\left(-\frac{r}{n}\right)} \left(\frac{2\,r}{n}\right)^l \mathrm{altLaguerreL}\left(n+l,\, 2\,l+1,\, \frac{2\,r}{n}\right)}{n^2}$$

```
> factor(expand(R(1, 0, r)));
```

$$\frac{2}{e^r}$$

```
> factor(expand(R(2, 0, r)));
```

$$-\frac{1}{4}\sqrt{2}\, e^{\left(-\frac{r}{2}\right)} (-2+r)$$

```
> factor(expand(R(2, 1, r)));
```

$$\frac{1}{12}\sqrt{6}\, e^{\left(-\frac{r}{2}\right)} r$$

[4] Our definition of ρ conforms to equation (16.32), but some authors have used $\rho = \frac{2r}{na_0}$.

```
> factor(expand(R(3, 0, r)));
```

$$\frac{2}{243}\sqrt{3}\,e^{(-\frac{r}{3})}\,(27-18\,r+2\,r^2)$$

```
> factor(expand(R(3, 1, r)));
```

$$-\frac{2}{243}\,r\,\sqrt{6}\,e^{(-\frac{r}{3})}\,(-6+r)$$

```
> factor(expand(R(3, 2, r)));
```

$$\frac{2}{1215}\sqrt{30}\,e^{(-\frac{r}{3})}\,r^2$$

```
> factor(expand(R(4, 0, r)));
```

$$-\frac{1}{768}\,e^{(-\frac{r}{4})}\,(-192+144\,r-24\,r^2+r^3)$$

```
> factor(expand(R(4, 1, r)));
```

$$\frac{1}{3840}\sqrt{15}\,e^{(-\frac{r}{4})}\,r\,(80-20\,r+r^2)$$

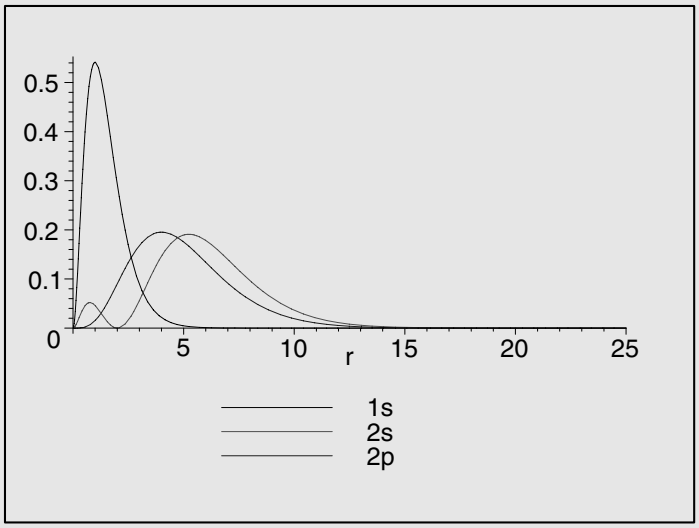
```
> factor(expand(R(4, 2, r)));
```

$$-\frac{1}{3840}\,r^2\,\sqrt{5}\,e^{(-\frac{r}{4})}\,(-12+r)$$

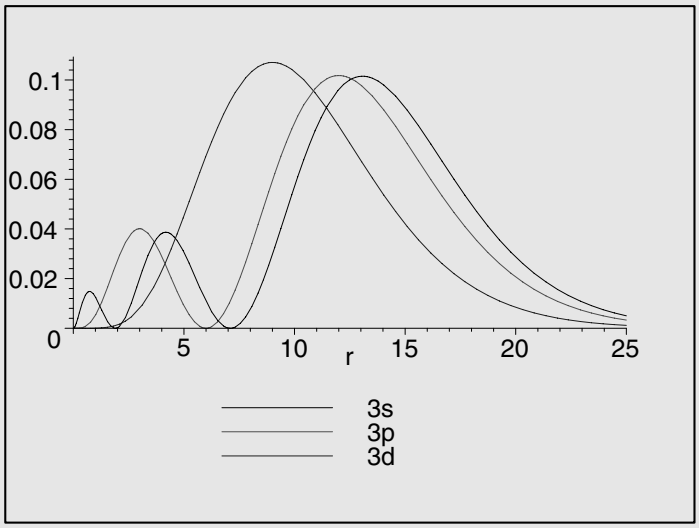
```
> factor(expand(R(4, 3, r)));
```

$$\frac{1}{26880}\sqrt{35}\,e^{(-\frac{r}{4})}\,r^3$$

```
> plot([R(1,0,r)^2*r^2, R(2,0,r)^2*r^2, R(2,1,r)^2*r^2], r=0..25,
> legend=["1s", "2s", "2p"]);
```



```
> plot([R(3,0,r)^2*r^2, R(3,1,r)^2*r^2, R(3,2,r)^2*r^2], r=0..25,
> legend=["3s", "3p", "3d"]);
```




```
> plot([R(4,0,r)^2*r^2, R(4,1,r)^2*r^2, R(4,2,r)^2*r^2,
> R(4,3,r)^2*r^2], r=0..40, legend=["4s", "4p", "4d", "4f"]);
```

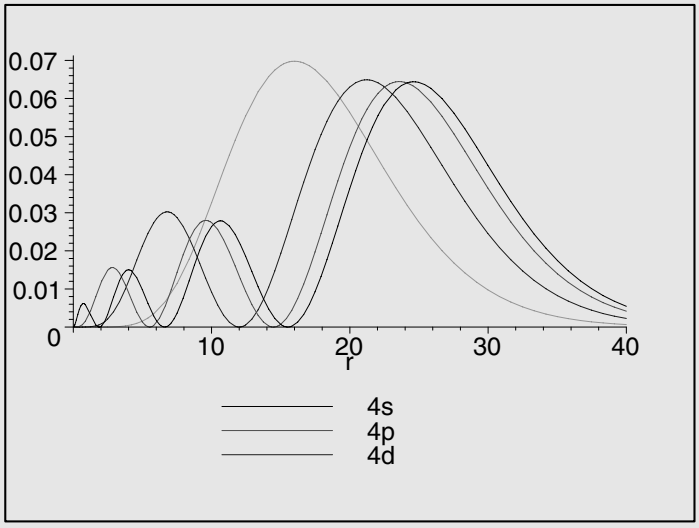


Table 16.2: Functions $R_{nl}(\rho)$. A constant factor $a_0^{-3/2}$ is omitted for each function.

n	l	$R_{nl}(\rho)$
1	0	$2e^{-\rho}$
2	0	$\frac{1}{\sqrt{2}}e^{-\rho/2}\left(1-\frac{1}{2}\rho\right)$
2	1	$\frac{1}{2\sqrt{6}}e^{-\rho/2}\rho$
3	0	$\frac{2}{3\sqrt{3}}e^{-\rho/3}\left(1-\frac{2}{3}\rho+\frac{2}{27}\rho^2\right)$
3	1	$\frac{8}{27\sqrt{6}}e^{-\rho/3}r\left(1-\frac{1}{6}\rho\right)$
3	2	$\frac{4}{81\sqrt{30}}e^{-\rho/3}\rho^2$
4	0	$\frac{1}{4}e^{-\rho/4}\left(1-\frac{3}{4}\rho+\frac{1}{8}\rho^2-\frac{1}{192}\rho^3\right)$
4	1	$\frac{5}{16\sqrt{15}}e^{-\rho/4}\rho\left(1-\frac{1}{4}+\frac{1}{80}\rho^2\right)$
4	2	$\frac{1}{64\sqrt{5}}e^{-\rho/4}\rho^2\left(1-\frac{1}{12}\rho\right)$
4	3	$\frac{1}{768\sqrt{35}}e^{-\rho/4}\rho^3$

We list wave functions for the first few states in Table 16.2. According to a postulate of quantum mechanics, the absolute square, or the product of wave function $\psi(r,\theta,\phi)$ with its complex conjugate, is interpreted as the probability density. The radial probability density is $|R_{nl}(r)|^2 r^2$, where a factor r^2 arises from the volume element in spherical coordinates:

$$d\tau = r^2 \sin\theta \, d\theta \, d\phi. \tag{16.46}$$

We plot the radial probability densities in the above worksheet, and the labels of these functions will be explained below. We observe that the number of nodes, excluding the origin, for $R_{nl}(r)$ is $n_r = n - l - 1$, the value of the radial quantum number.

We can also plot the angular dependence of the probability density functions, which are the squares of the spherical harmonics $|Y_{lm}(\theta,\phi)|^2$.

Worksheet 16.4 We plot $|Y_{lm}(\theta,\phi)|^2$ for $l = 1, 2, 3$. Although we type in these spherical harmonics, they can be derived by Maple, as demonstrated in the worksheet in Section 16.2. It is trivial to prove that $|Y_{lm}(\theta,\phi)|^2$ has no azimuthal dependence (the function contains no ϕ). For each plot, we obtain a surface of revolution about the z axis. For each l we also plot a combination

$$\sum_{m=-l-1}^{l+1} |Y_{lm}(\theta,\phi)|^2;$$

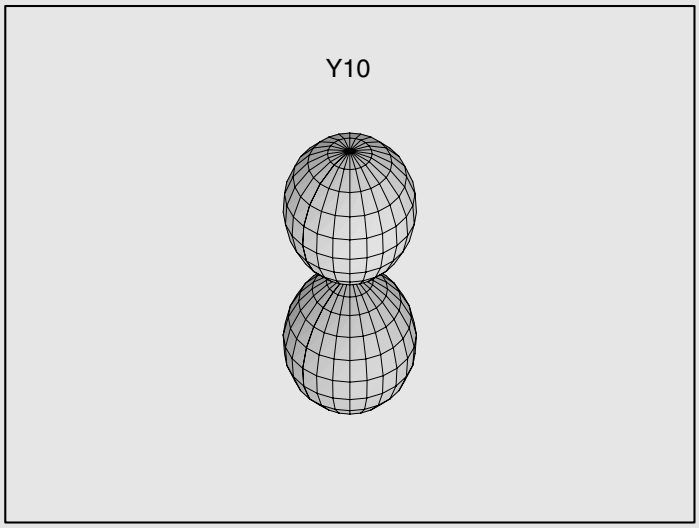
from these graphs such a combination clearly results in spherical symmetry, which is an indication that the function does not depend on θ or ϕ.

```
> assume(phi, real):

> Y10 := sqrt(3/(4*Pi))*cos(theta);
```

$$Y10 := \frac{1}{2}\,\frac{\sqrt{3}\cos(\theta)}{\sqrt{\pi}}$$

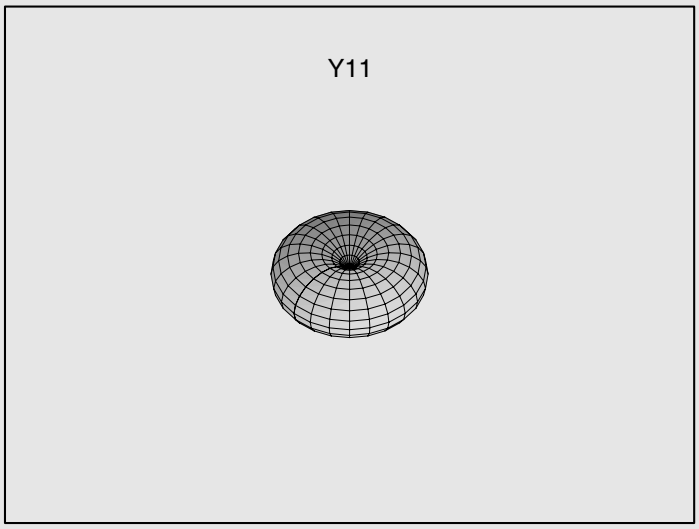
```
> plot3d(Y10*conjugate(Y10), phi=0..2*Pi, theta=0..Pi,
> coords=spherical, scaling=constrained, view=-0.25..0.25,
> title="Y10");
```



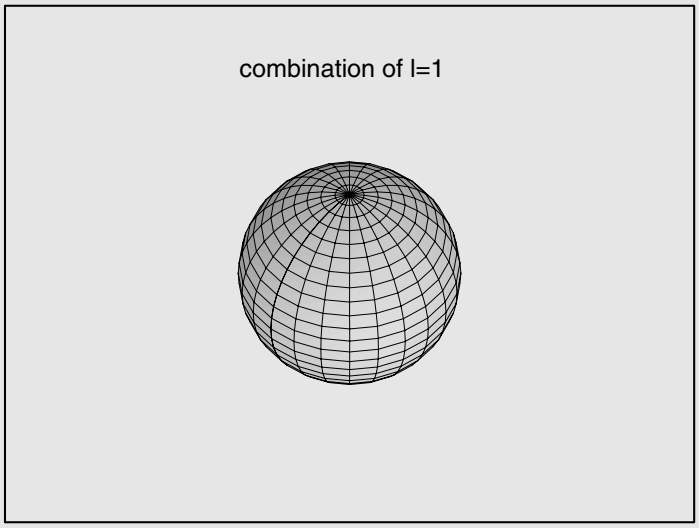

```
> Y11 := -sqrt(3/(8*Pi))*sin(theta)*exp(I*phi);
```

$$Y11 := -\frac{1}{4}\,\frac{\sqrt{6}\sin(\theta)\,e^{(\phi\,I)}}{\sqrt{\pi}}$$

```
> plot3d(Y11*conjugate(Y11), phi=0..2*Pi, theta=0..Pi,
> coords=spherical, scaling=constrained, view=-0.25..0.25,
> title="Y11");
```



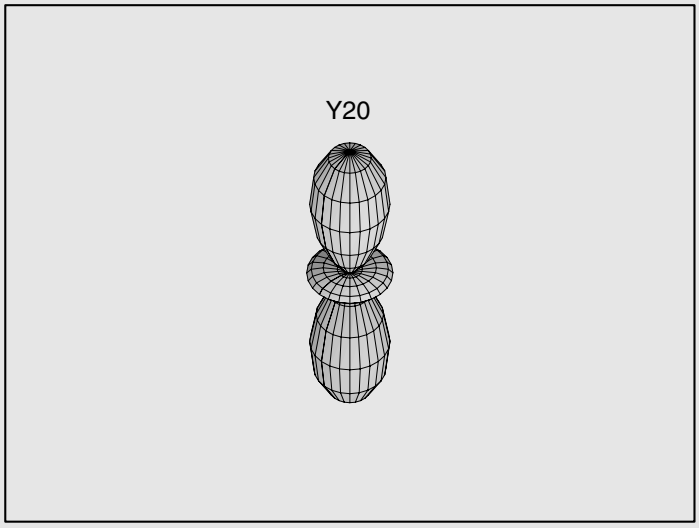

```
> plot3d(Y10*conjugate(Y10) + 2*Y11*conjugate(Y11), phi=0..2*Pi,
> theta=0..Pi, coords=spherical, scaling=constrained,
view=-0.25..0.25,
> title="combination of l=1");
```




```
> Y20 := sqrt(5/(16*Pi))*(3*cos(theta)^2 -1);
```

$$Y20 := \frac{1}{4}\,\frac{\sqrt{5}\,(3\cos(\theta)^2-1)}{\sqrt{\pi}}$$

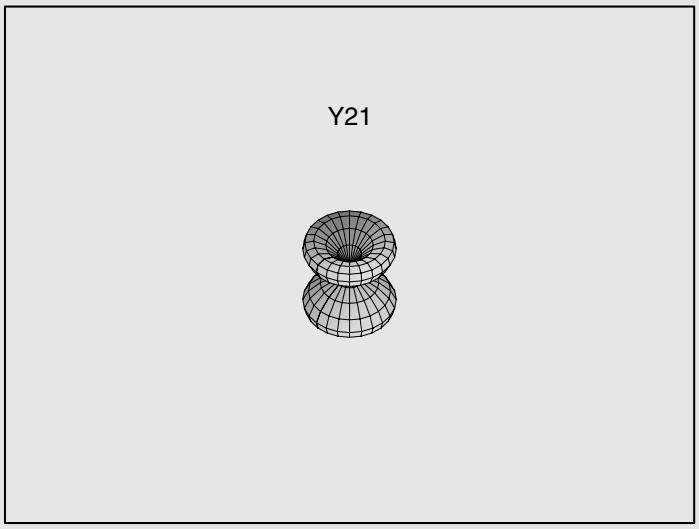
```
> plot3d(Y20*conjugate(Y20), phi=0..2*Pi, theta=0..Pi,
> coords=spherical, scaling=constrained, view=-0.5..0.5,
> title="Y20");
```




```
> Y21 := -sqrt(15/(8*Pi))*sin(theta)*cos(theta)*exp(I*phi);
```

$$Y21 := -\frac{1}{4}\,\frac{\sqrt{30}\sin(\theta)\cos(\theta)\,e^{(\phi\,I)}}{\sqrt{\pi}}$$

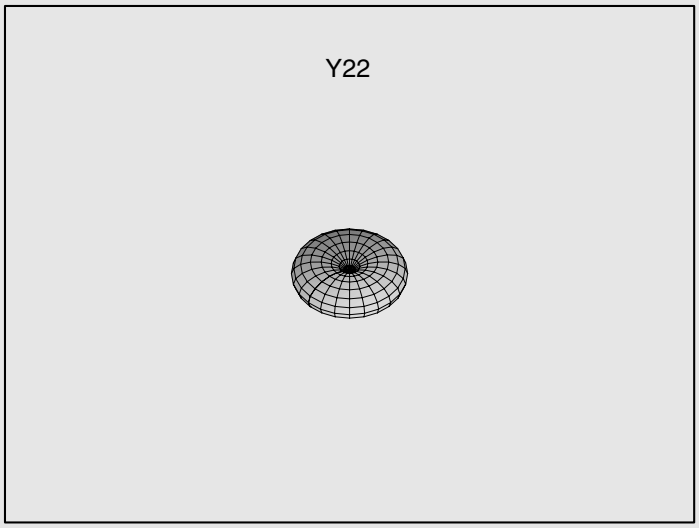
```
> plot3d(Y21*conjugate(Y21), phi=0..2*Pi, theta=0..Pi,
> coords=spherical, scaling=constrained, view=-0.5..0.5,
> title="Y21");
```



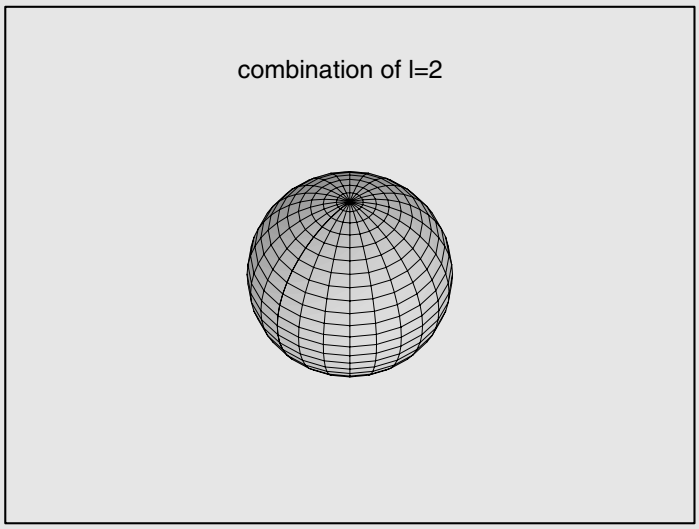

```
> Y22 := sqrt(15/(32*Pi))*sin(theta)^2*exp(2*I*phi);
```

$$Y22 := \frac{1}{8}\,\frac{\sqrt{30}\sin(\theta)^2\,e^{(2\,I\,\phi)}}{\sqrt{\pi}}$$

```
> plot3d(Y22*conjugate(Y22), phi=0..2*Pi, theta=0..Pi,
> coords=spherical, scaling=constrained, view=-0.5..0.5,
> title="Y22");
```



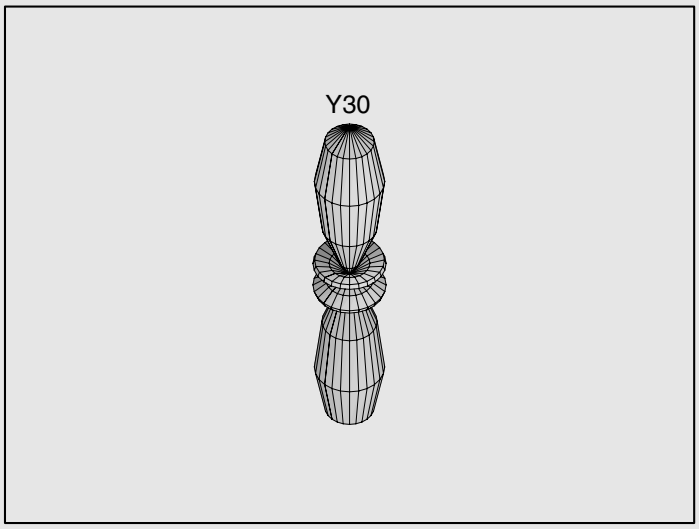
```
> plot3d(Y20*conjugate(Y20) +  2*Y21*conjugate(Y21) +
> 2*Y22*conjugate(Y22), phi=0..2*Pi, theta=0..Pi, coords=spherical,
> scaling=constrained, view=-0.5..0.5, title="combination of l=2");
```




```
> Y30 := sqrt(7/(16*Pi))*(5*cos(theta)^3 - 3*cos(theta));
```

$$Y30 := \frac{1}{4}\,\frac{\sqrt{7}\,(5\cos(\theta)^3 - 3\cos(\theta))}{\sqrt{\pi}}$$

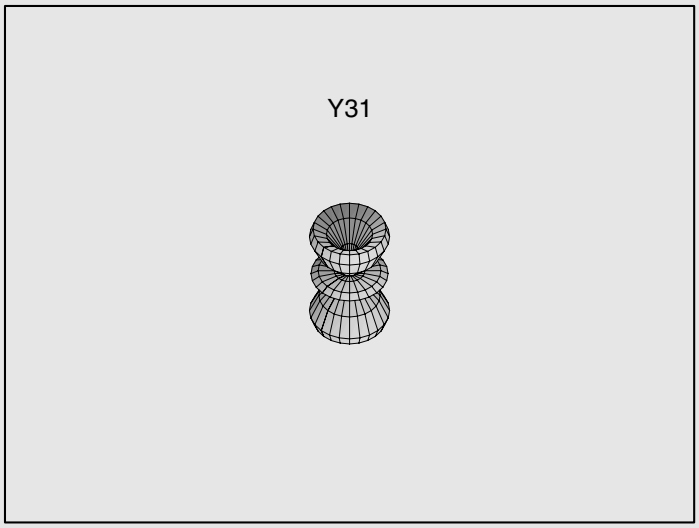
```
> plot3d(Y30*conjugate(Y30), phi=0..2*Pi, theta=0..Pi,
> coords=spherical, scaling=constrained, view=-0.6..0.6,
> title="Y30");
```




```
> Y31 := -sqrt(21/(64*Pi))*(5*cos(theta)^2 -
> 1)*sin(theta)*exp(I*phi);
```

$$Y31 := -\frac{1}{8}\,\frac{\sqrt{21}\,(5\cos(\theta)^2-1)\sin(\theta)\,e^{(\phi\,I)}}{\sqrt{\pi}}$$

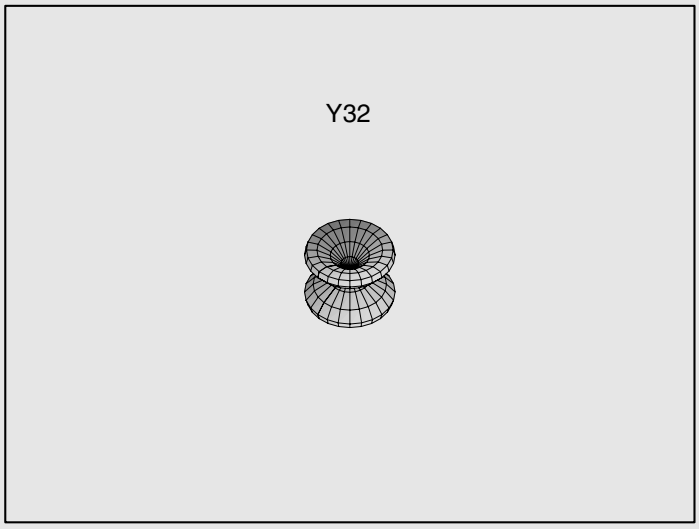
```
> plot3d(Y31*conjugate(Y31), phi=0..2*Pi, theta=0..Pi,
> coords=spherical, scaling=constrained, view=-0.6..0.6,
> title="Y31");
```



```
> Y32 := sqrt(210/(64*Pi))*cos(theta)*sin(theta)^2*exp(2*I*phi);
```

$$Y32 := \frac{1}{8}\,\frac{\sqrt{210}\cos(\theta)\sin(\theta)^2\,e^{(2\,I\,\phi)}}{\sqrt{\pi}}$$

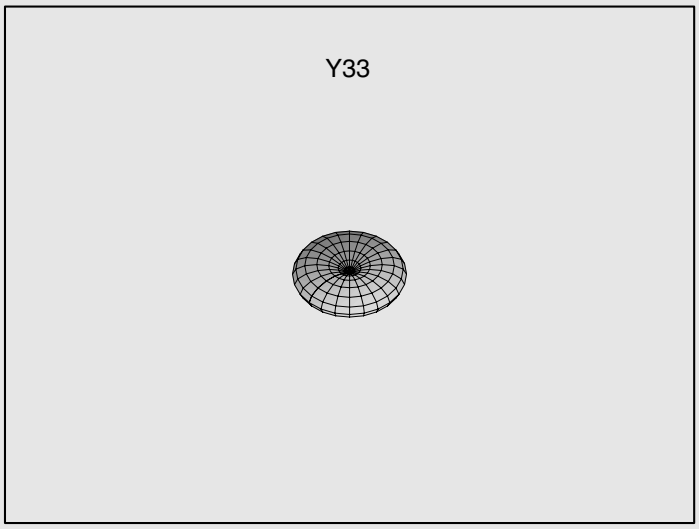
```
> plot3d(Y32*conjugate(Y32), phi=0..2*Pi, theta=0..Pi,
> coords=spherical, scaling=constrained, view=-0.6..0.6,
> title="Y32");
```



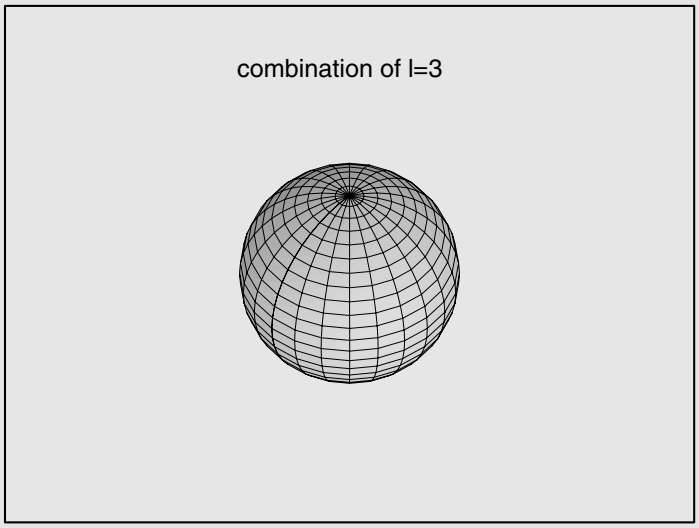

```
> Y33 := -sqrt(35/(64*Pi))*sin(theta)^3*exp(3*I*phi);
```

$$Y33 := -\frac{1}{8}\,\frac{\sqrt{35}\sin(\theta)^3\,e^{(3\,I\,\phi)}}{\sqrt{\pi}}$$

```
> plot3d(Y33*conjugate(Y33), phi=0..2*Pi, theta=0..Pi,
> coords=spherical, scaling=constrained, view=-0.6..0.6,
> title="Y33");
```




```
> plot3d(Y30*conjugate(Y30) + 2*Y31*conjugate(Y31) +
> 2*Y32*conjugate(Y32) + 2*Y33*conjugate(Y33), phi=0..2*Pi,
theta=0..Pi,
> coords=spherical, scaling=constrained, view=-0.6..0.6,
> title="combination of l=3");
```



In summary, the complete wave function for the hydrogen atom is the product of the radial and angular parts:

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi), \tag{16.47}$$

where $R_{nl}(r)$ is the associated Laguerre function and $Y_{lm}(\theta,\phi)$ the spherical harmonics, both well defined special functions. To represent a quantum state, a particular wave function is characterized by three quantum numbers: the principal quantum number n, the quantum number for the total angular momentum l, and the magnetic quantum number m. The energy of a quantum state is determined solely by the principal quantum n, which is a property unique to the Coulomb potential. The energy of each discrete state is identical to that based on Bohr's model:

$$H\psi_{nlm} = -\frac{1}{n^2}\frac{\mu e^4}{8h^2\epsilon_0^2}\psi_{nlm}. \tag{16.48}$$

This wave function is also the eigenfunction of the square of angular momentum, and the eigenvalue is $l(l+1)$,

$$L^2\psi_{nlm} = l(l+1)\hbar^2\psi_{nlm}. \tag{16.49}$$

Furthermore, the wave function is the eigenfunction of the projection of the angular momentum on one axis, commonly taken to be z, and the eigenvalue is $m\hbar$,

$$L_z\psi_{nlm} = m\hbar\psi_{nlm}. \tag{16.50}$$

For a given n, the possible range of l is from 0 to $n-1$; for given l, the possible range of m is from $-l$ to $+l$. A notation for states with various values of quantum number l for angular momentum is

$$\begin{array}{cccccccccc} l & = & 0 & 1 & 2 & 3 & 4 & 5 & \ldots \\ & & s & p & d & f & g & h & \ldots \end{array}$$

The common method of labeling a wave function of n and l involves a number to specify a value of the principal quantum number n, followed by a letter to specify a value of l, according to the above correlation; for instance, $4d$ denotes a wave function with $n=4$ and $l=2$.

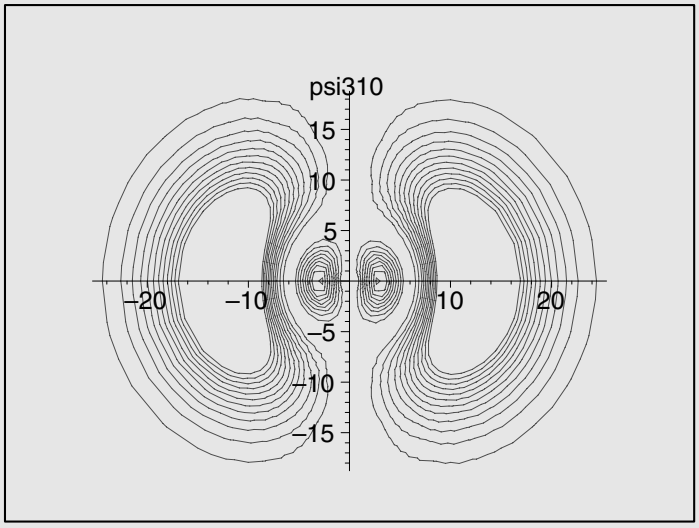
We plot the functions of probability density, which are the absolute squares of the complete wave functions for the hydrogen atom.

Worksheet 16.5 In this worksheet, we plot, as examples, three probability density functions for the hydrogen atom: $|\psi_{310}(r,\theta,\phi)|^2$, $|\psi_{320}(r,\theta,\phi)|^2$, $|\psi_{321}(r,\theta,\phi)|^2$. The probability density function has no azimuthal dependence as it contains no ϕ term. Similar to the plot of equipotential surface, we visualize a function of two variables using the `implicitplot` command. We graph each surface that corresponds to a particular value of probability. We also employ the `implicitplot3d` command to plot the probability density function for $|\psi_{430}(r,\theta,\phi)|^2$, which is a surface of revolution. Be aware that, when using polar coordinates in a two-dimensional plot, θ is measured with respect to the x axis, whereas, when using spherical coordinates in a three-dimensional plot, θ is measured with respect to the z axis; the x axis in a polar plot therefore corresponds to the z axis in the spherical plot.

```
> assume(phi, real):
> with(plots):
Warning, the name changecoords has been redefined
> psi310 := 8/(27*sqrt(6))*exp(-r/3)*r*(1 -
> r/6)*sqrt(3/(4*Pi))*cos(theta);
```

$$\psi 310 := \frac{2}{81}\,\frac{\sqrt{6}\,e^{(-\frac{r}{3})}\,r\,\left(1-\frac{r}{6}\right)\,\sqrt{3}\cos(\theta)}{\sqrt{\pi}}$$

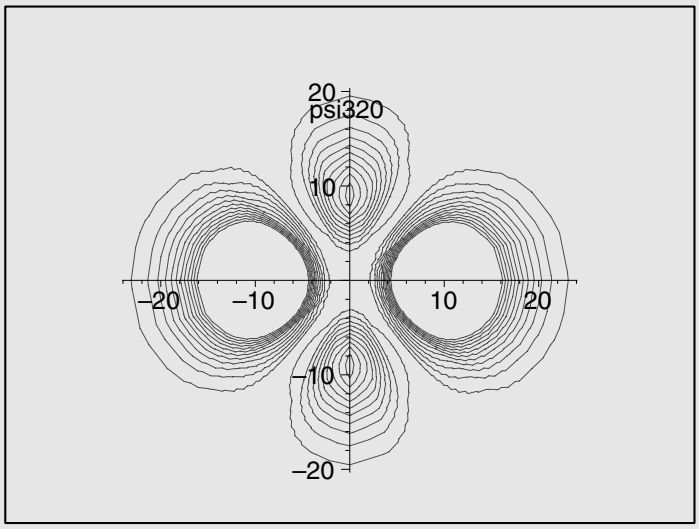
```
> implicitplot({seq(r^2*psi310*conjugate(psi310)=0.001*i,
> i=1..12)}, r=0..25, theta=0..2*Pi, coords=polar,
> scaling=constrained, numpoints=800, title="psi310");
```




```
> psi320 :=
> 4/(81*sqrt(30))*exp(-r/3)*r^2*sqrt(5/(16*Pi))*(3*cos(theta)^2 -
1);
```

$$\psi 320 := \frac{1}{2430}\,\frac{\sqrt{30}\,e^{(-\frac{r}{3})}\,r^2\,\sqrt{5}\,(3\cos(\theta)^2-1)}{\sqrt{\pi}}$$

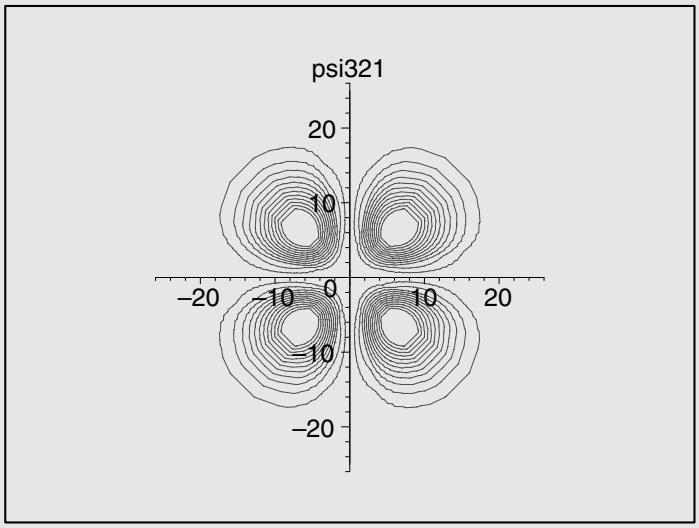
```
> implicitplot({seq(r^2*psi320*conjugate(psi320)=0.001*i,
> i=1..12)}, r=0..25, theta=0..2*Pi, coords=polar,
> scaling=constrained, numpoints=800, title="psi320");
```




```
> psi321 :=
> 4/(81*sqrt(30))*exp(-r/3)*r^2*(-sqrt(15/(8*Pi)))*sin(theta)
> *cos(theta)*exp(I*phi);
```

$$\psi 321 := -\frac{1}{81}\,\frac{e^{(-\frac{r}{3})}\,r^2\sin(\theta)\cos(\theta)\,e^{(\phi\,I)}}{\sqrt{\pi}}$$

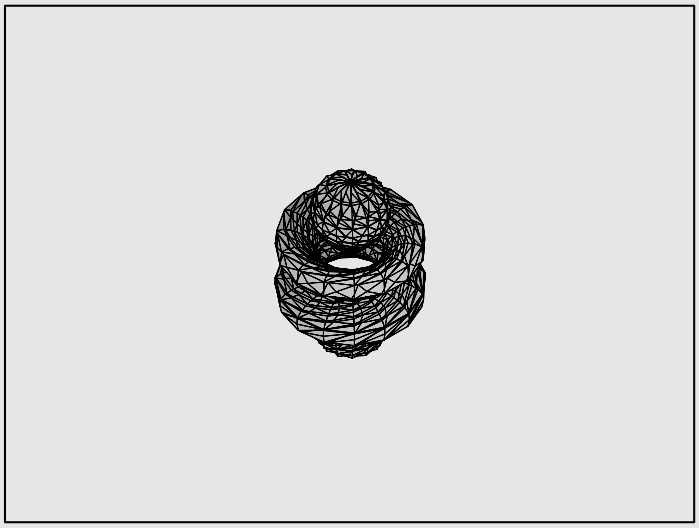
```
> implicitplot({seq(r^2*psi321*conjugate(psi321)=.001*i, i=0..12)},
> r=0..25, theta=0..2*Pi, coords=polar, scaling=constrained,
> numpoints=800, title="psi321");
```



```
> psi430 :=
> 1/(768*sqrt(35))*exp(-r/4)*r^3*sqrt(7/(16*Pi))*(5*cos(theta)^3 -
> 3*cos(theta));
```

$$\psi 430 := \frac{1}{107520}\,\frac{\sqrt{35}\,e^{(-\frac{r}{4})}\,r^3\,\sqrt{7}\,(5\cos(\theta)^3 - 3\cos(\theta))}{\sqrt{\pi}}$$

```
> implicitplot3d(r^2*psi430*conjugate(psi430)=0.004, r=0..32,
> phi=0..2*Pi, theta=0..Pi, coords=spherical, grid=[16, 16, 16],
> scaling=constrained);
```



When we view these two-dimensional plots, we must understand that they are rotated by 90° from the three-dimensional plots.

Wave functions are a powerful tool in quantum mechanics; the most notable success is that the constraint of a wave function to remain finite yields quantization of energy and angular momentum, which is an inevitable consequence from purely mathematical properties of the wave functions based on reasonable assumptions. We form plots of the probability functions related to these wave functions in order to visualize them. Misinterpretation of these plots is an unfortunate side effect; many students mistakenly consider atoms to look like blobs, lobes and dumb-bells depicted in the preceding worksheet. We emphasize that plots of probability functions are *not* experimentally observable on atoms in the absence of external magnetic or electric fields. We know that, for instance, these five solutions ψ_{322}, ψ_{321}, ψ_{320}, ψ_{32-1}, ψ_{32-2} correspond to a single energy in absence of external fields because they are degenerate states.

We can only observe their combination, which is spherically symmetric as shown in an earlier worksheet.

It is impossible to obtain exact solutions for a multi-electron atom, which is one instance of a many-body problem; approximations must be devised. According to Hartree's method, electrons move independently in a spherically symmetric net potential $V(r)$ which takes into account charges of the nucleus and all other electrons. The determination of the net potential $V(r)$ requires an iterative process involving trial and modification. Eventually, one finds a self-consistent potential $V(r)$ that yields energies that conform to experimental measurements of their differences.

Because this self-consistent potential is spherically symmetric, the angular dependence of the wave functions is the same as for the hydrogen atom, with labels s, p, d, f, and so on, and with various possible values of m. For the radial part one uses the self-consistent potential $V(r)$ and solves the equation numerically. The shapes of the wave functions qualitatively resemble those for the hydrogen atom: the number of nodes is just $n_r = n - l - 1$. We therefore adopt the same notation to denote a solution that pertains to each quantum state, such as $4d$ and $2p$. However, under the self-consistent potential, states with the same n but different l are no longer degenerate; greater l implies greater energy. According to this model, the energy of a state associated with $4s$ is less than that for $3d$, and analogously that for $5s$ is less than that for $4d$.

An electron has spin $\frac{1}{2}\hbar$; it thus obeys Pauli's exclusion principle: two electrons can never be in the same quantum state. For given l, the number m takes $2l + 1$ values, and the number of possible electron spin orientations is 2. Therefore, there are in total $2(2l + 1)$ different states allowed with the same n and l.

Table 16.3: Atomic energy levels.

$1s$	2
$2s$, $2p$	8
$3s$, $3p$	8
$4s$, $3d$, $4p$	18
$5s$, $4d$, $5p$	18
$6s$, $4f$, $5d$, $6p$	32

In Table 16.3, we list the results of Hartree's approximate method. Quantum states are grouped in approximate order of energy, and between each row there are significant gaps. An ensemble of electrons encompassing all possible values of each row in this table corresponds to atomic numbers 2, 10, 18, 36, 54 and 86, or noble gases helium, neon, argon, krypton, xenon and radon, respectively. We rationalize that these elements show little tendency to form chemical compounds because their ionization energies are the greatest in their respective series.

16.5.1 Electric Potential Due to the Electron

Using the wave functions, we can calculate the electric potential due to the electron in hydrogen. As an example, for the $m = \pm 1$ states in the $2p$ level in hydrogen, the charge density is

$$\rho(\mathbf{r}_2) = q\psi^*_{211}\psi_{211} = \frac{q}{64\pi}\frac{r_2^2}{a_0^5}e^{-r_2/a_0}\sin^2\theta_2. \tag{16.51}$$

The potential is obtainable from the integral

$$V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0}\int\frac{\rho(\mathbf{r}_2)}{r_{12}}d\tau_2. \tag{16.52}$$

In equation (16.21), the length of the separation vector r_{12}^{-1} is expanded in terms of spherical harmonics:

$$\frac{1}{r_{12}} = \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{1}{2l+1}\frac{r_<^l}{r_>^{l+1}}Y^*_{lm}(\theta_2,\phi_2)Y_{lm}(\theta_1,\phi_1). \tag{16.21}$$

We can thus write the potential as a multipole expansion,

$$V(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}C_{lm}Y_{l,m}(\theta_1,\phi_1), \tag{16.53}$$

where

$$C_{lm} = \int Y^*_{lm}(\theta_2,\phi_2)\frac{r_<^l}{r_>^{l+1}}\rho(\mathbf{r}_2)\,d\tau_2. \tag{16.54}$$

Because we are dealing with an extended charge distribution, we split the integral into two parts: first from 0 to r_1 for $r_1 \geq r_2$, then from r_1 to ∞ for $r_1 \leq r_2$. Explicitly, we list the first two nonvanishing terms:

$$C_{00} = 2\pi\left[\int_0^{r_1} dr_2\int_0^{\pi} d\theta_2\rho(\mathbf{r}_2)\frac{1}{r_1}r_2^2\sin\theta_2 + \int_{r_1}^{\infty} dr_2\int_0^{\pi} d\theta_2\rho(\mathbf{r}_2)\frac{1}{r_2}r_2^2\sin\theta_2\right], \tag{16.55}$$

$$C_{20} = 2\pi\left[\int_0^{r_1} dr_2\int_0^{\pi} d\theta_2\rho(\mathbf{r}_2)\frac{r_2^2}{r_1^3}r_2^2\sin\theta_2 + \int_{r_1}^{\infty} dr_2\int_0^{\pi} d\theta_2\rho(\mathbf{r}_2)\frac{r_1^2}{r_2^3}r_2^2\sin\theta_2\right]. \tag{16.56}$$

The integral is elementary, but involves tedious algebra. We refer the reader to the Maple worksheet below for the long result. For small r_1, expanding V near the origin yields

$$V(\mathbf{r}_1) = \frac{q}{4\pi\epsilon_0 a}\left[\frac{1}{4} - \frac{r_1^2}{120a^2}\left(\frac{3}{2}\cos^2\theta_1 - \frac{1}{2}\right)\right]. \tag{16.57}$$

This potential is useful in calculating the interaction energy between the nuclear quadrupole moment and electronic charge.[5]

Worksheet 16.6 It is straightforward to enter these integrals for Maple to evaluate. For complicated integrands, it is helpful to use `Int` and `value` in a pair, so that one can see the integrands, to avoid typographical errors.

```
> assume(a>0):
> den := q/a^5*1/(64*Pi)*r2^2*exp(-r2/a)*sin(theta2)^2;
```

$$den := \frac{1}{64}\frac{q\,r2^2\,e^{(-\frac{r2}{a})}\sin(\theta2)^2}{a^5\,\pi}$$

```
> Y00 := 1/sqrt(4*Pi);
```

$$Y00 := \frac{1}{2\sqrt{\pi}}$$

```
> Y20 := sqrt(5/(4*Pi))*(3/2*cos(theta)^2 - 1/2);
```

$$Y20 := \frac{1}{2}\frac{\sqrt{5}\left(\frac{3}{2}\cos(\theta)^2 - \frac{1}{2}\right)}{\sqrt{\pi}}$$

```
> 2*Pi*(Int(Int(den*Y00*r2^2*sin(theta2)/r1, theta2=0..Pi),
> r2=0..r1) + Int(Int(den*Y00*r2*sin(theta2), theta2=0..Pi),
> r2=r1..infinity));
```

$$2\,\pi\left(\int_0^{r1}\int_0^{\pi}\frac{1}{128}\frac{q\,r2^4\,e^{(-\frac{r2}{a})}\sin(\theta2)^3}{a^5\,\pi^{(3/2)}\,r1}\,d\theta2\,dr2 + \int_{r1}^{\infty}\int_0^{\pi}\frac{1}{128}\frac{q\,r2^3\,e^{(-\frac{r2}{a})}\sin(\theta2)^3}{a^5\,\pi^{(3/2)}}\,d\theta2\,dr2\right)$$

```
> C00 := value(%):
```

[5] Jackson 1999, problem 4.7, p. 171.

```
> 2*Pi*(Int(Int(den*r2^2/r1^3*eval(Y20, theta=theta2)*sin(theta2)
> *r2^2, theta2=0..Pi), r2=0..r1) + Int(Int(den*r1^2/r2^3*eval(Y20,
> theta=theta2)*sin(theta2)*r2^2, theta2=0..Pi), r2=r1..infinity));
```

$$2\,\pi\left(\int_0^{r1}\int_0^{\pi}\frac{1}{128}\,\frac{q\,r2^6\,e^{(-\frac{r2}{a})}\sin(\theta2)^3\,\sqrt{5}\,\left(\frac{3}{2}\cos(\theta2)^2-\frac{1}{2}\right)}{a^5\,\pi^{(3/2)}\,r1^3}\,d\theta2\,dr2\right.$$

$$\left.+\int_{r1}^{\infty}\int_0^{\pi}\frac{1}{128}\,\frac{q\,r2\,e^{(-\frac{r2}{a})}\sin(\theta2)^3\,r1^2\,\sqrt{5}\,\left(\frac{3}{2}\cos(\theta2)^2-\frac{1}{2}\right)}{a^5\,\pi^{(3/2)}}\,d\theta2\,dr2\right)$$

```
> C20 := value(%):
> V := 1/epsilon[0]*(simplify(C00)*Y00 + 1/5*simplify(C20)*eval(Y20,
> theta=theta1));
```

$$V := \left(\frac{1}{96}\,\frac{q\,(-18\,r1\,a^2-24\,a^3-6\,r1^2\,a-r1^3+24\,e^{(\frac{r1}{a})}\,a^3)\,e^{(-\frac{r1}{a})}}{\pi\,a^3\,r1}-\frac{1}{96}q\right.$$

$$(-24\,a^2\,r1^3-144\,a^5-72\,a^3\,r1^2-6\,a\,r1^4-144\,a^4\,r1-r1^5+144\,e^{(\frac{r1}{a})}\,a^5)\,e^{(-\frac{r1}{a})}$$

$$\left.\left(\frac{3}{2}\cos(\theta1)^2-\frac{1}{2}\right)\Big/(\pi\,a^3\,r1^3)\right)\Big/\varepsilon_0$$

```
> taylor(V, r1);
```

$$\frac{1}{16}\,\frac{q}{\varepsilon_0\,\pi\,a}-\frac{1}{480}\,\frac{q\,\left(\frac{3}{2}\cos(\theta1)^2-\frac{1}{2}\right)}{\varepsilon_0\,\pi\,a^3}\,r1^2+\mathrm{O}(r1^3)$$

16.5.2 Hybrid Bond Orbitals

Wave functions for a hydrogen atom also serve as a basis for calculations in quantum chemistry. The term *orbital* refers to a solution of the Schrödinger equation for a system of only one electron. The linear combination of orbitals is used to model the directional properties of the chemical bond, which Linus Pauling made an important contribution.

To eliminate the complex character of wave functions so as to retain only the real parts, one can linearly combine the angular part of spherical harmonics $Y_{lm}(\theta,\phi)$ using Euler's formula.

For example, for $l = 1$, we construct the p_x, p_y and p_z solutions as, neglecting a factor $1/\sqrt{4\pi}$,

$$\begin{array}{lll} p_z & = Y_{10}(\theta,\phi) & = \sqrt{3}\cos\theta, \\ p_x & = \frac{1}{\sqrt{2}}[Y_{1,1}(\theta,\phi) + Y_{1,-1}(\theta,\phi)] & = \sqrt{3}\sin\theta\cos\phi, \\ p_y & = \frac{1}{i\sqrt{2}}[Y_{1,1}(\theta,\phi) - Y_{1,-1}(\theta,\phi)] & = \sqrt{3}\sin\theta\sin\phi. \end{array} \tag{16.58}$$

Although this combination serves for approximate calculations on molecules such as H_2O and NH_3, it fails for organic compounds such as CH_4 and C_2H_4. For these molecules, one takes wave functions in other combinations involving disparate values of l, to form so-called "hybridized orbitals".

Worksheet 16.7 Assuming the radial dependences of wave functions with the same value of n, for example $2s$ and $2p$, to be similar, the basis wave functions that we employ are proportional to

$$s = 1, \quad p_x = \sqrt{3}\sin\theta\cos\phi, \quad p_y = \sqrt{3}\sin\theta\sin\phi, \quad p_z = \sqrt{3}\cos\theta.$$

We construct, in an obvious notation, four sp^3 hybridized orbitals,[6]

$$t_1 = \frac{1}{2}(s + p_x + p_y + p_z), \tag{16.59a}$$

$$t_2 = \frac{1}{2}(s + p_x - p_y - p_z), \tag{16.59b}$$

$$t_3 = \frac{1}{2}(s - p_x + p_y - p_z), \tag{16.59c}$$

$$t_4 = \frac{1}{2}(s - p_x - p_y + p_z). \tag{16.59d}$$

According to the plots, each function differs from another only by being rotated through $\arccos(-1/3) = 109°28'$. This combination is used to explain the tetrahedral structure of CH_4, methane.

We also plot the sp^2 hybridized orbital, which is

$$f_1 = \frac{1}{\sqrt{3}}(s + \sqrt{2}p_x), \tag{16.60a}$$

$$f_2 = \frac{1}{\sqrt{6}}(\sqrt{2}s - p_x + \sqrt{3}p_y), \tag{16.60b}$$

$$f_1 = \frac{1}{\sqrt{6}}(\sqrt{2}s - p_x - \sqrt{3}p_y), \tag{16.60c}$$

together with the unhybridized orbital p_z. Each of the sp^2 orbital differs from another by a rotation of $120°$. This combination serves to explain the structure of C_2H_4, ethene.

[6] L. Pauling, *General Chemistry*, New York: Dover Publications, 1988, p. 906

```
> s := 1; px := sqrt(3)*sin(theta)*cos(phi); py :=
> sqrt(3)*sin(theta)*sin(phi); pz := sqrt(3)*cos(theta);
```

$$s := 1$$

$$px := \sqrt{3}\sin(\theta)\cos(\phi)$$

$$py := \sqrt{3}\sin(\theta)\sin(\phi)$$

$$pz := \sqrt{3}\cos(\theta)$$

```
> t1 := 1/2*(s + px + py + pz); t2 := 1/2*(s + px - py - pz);
> t3 := 1/2*(s - px + py - pz); t4 := 1/2*(s - px - py + pz);
```

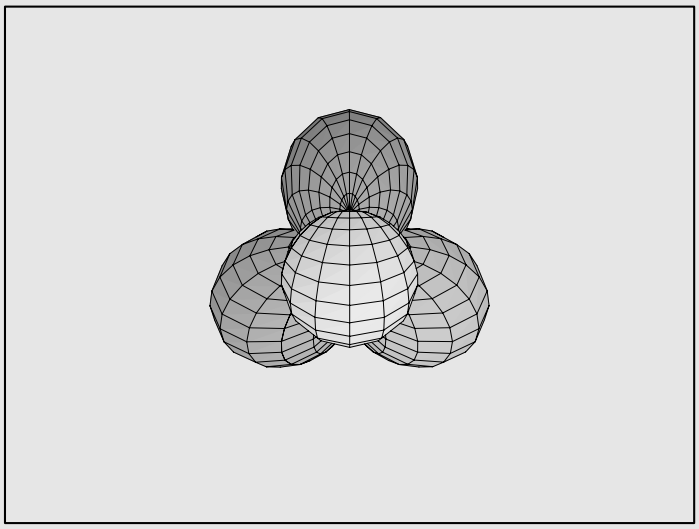
$$t1 := \frac{1}{2} + \frac{1}{2}\sqrt{3}\sin(\theta)\cos(\phi) + \frac{1}{2}\sqrt{3}\sin(\theta)\sin(\phi) + \frac{1}{2}\sqrt{3}\cos(\theta)$$

$$t2 := \frac{1}{2} + \frac{1}{2}\sqrt{3}\sin(\theta)\cos(\phi) - \frac{1}{2}\sqrt{3}\sin(\theta)\sin(\phi) - \frac{1}{2}\sqrt{3}\cos(\theta)$$

$$t3 := \frac{1}{2} - \frac{1}{2}\sqrt{3}\sin(\theta)\cos(\phi) + \frac{1}{2}\sqrt{3}\sin(\theta)\sin(\phi) - \frac{1}{2}\sqrt{3}\cos(\theta)$$

$$t4 := \frac{1}{2} - \frac{1}{2}\sqrt{3}\sin(\theta)\cos(\phi) - \frac{1}{2}\sqrt{3}\sin(\theta)\sin(\phi) + \frac{1}{2}\sqrt{3}\cos(\theta)$$

```
> plot3d({t1^2, t2^2, t3^2, t4^2}, phi=0..2*Pi, theta=0..Pi,
> coords=spherical, scaling=constrained);
```



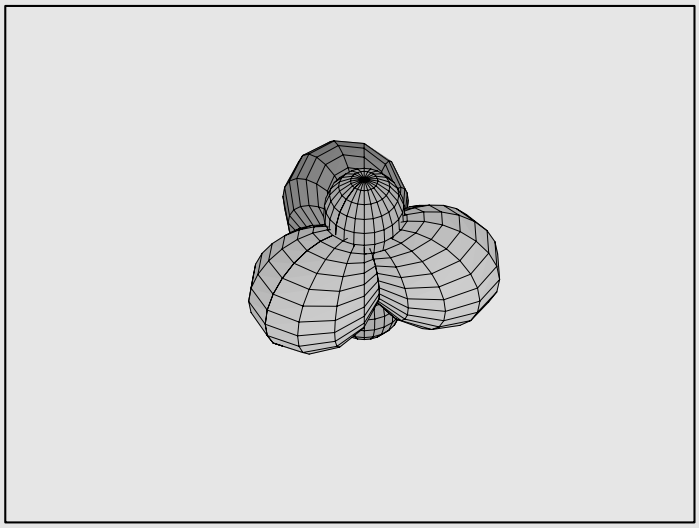
```
> f1 := 1/sqrt(3)*(s + sqrt(2)*px); f2 := 1/sqrt(6)*(sqrt(2)*s
> - px + sqrt(3)*py); f3 := 1/sqrt(6)*(sqrt(2)*s - px -sqrt(3)*py);
```

$$f1 := \frac{1}{3}\sqrt{3}\left(1 + \sqrt{2}\sqrt{3}\sin(\theta)\cos(\phi)\right)$$

$$f2 := \frac{1}{6}\sqrt{6}\,(\sqrt{2} - \sqrt{3}\sin(\theta)\cos(\phi) + 3\sin(\theta)\sin(\phi))$$

$$f3 := \frac{1}{6}\sqrt{6}\,(\sqrt{2} - \sqrt{3}\sin(\theta)\cos(\phi) - 3\sin(\theta)\sin(\phi))$$

```
> plot3d({f1^2, f2^2, f3^2, pz^2}, phi=0..2*Pi, theta=0..Pi,
> coords=spherical, scaling=constrained);
```



The above plots are again *not* physically observable. Although quantum mechanics in principle enables us to calculate chemical properties of matter, the labor that must go into such calculations, if possible, is often far greater than that which would be required to make an experimental study. Semiempirical calculations are usually complex and tedious, and most knowledge of chemical properties still comes from experience and experiment, rather than quantum calculations.

16.6 Infinite Spherical Well

We consider an infinite spherical well, described by

$$V(r) = \begin{cases} 0, & r < a, \\ \infty, & r > a. \end{cases} \tag{16.61}$$

Because this potential is spherically symmetric, the angular part of the solution of the three-dimensional Schrödinger equation is simply the spherical harmonics $Y_{lm}(\theta, \phi)$; we hence only

consider the solution of the radial equation. For $r < a$, because $V(r) = 0$, the radial equation is

$$-\frac{\hbar^2}{2\mu r^2}\frac{d}{dr}\left[r^2\frac{dR(r)}{dr}\right] + \frac{l(l+1)\hbar^2}{2\mu r^2}R(r) = ER(r). \tag{16.62}$$

We use Maple to solve this equation directly.

Worksheet 16.8

```
> assume(l, posint):
> Eq1 := -h_^2/(2*mu*r^2)*diff(r^2*diff(R(r), r), r) +
> (l*(l+1)*h_^2/(2*mu*r^2))*R(r) = En*R(r);
```

$$Eq1 := -\frac{1}{2}\frac{h_^2\,(2\,r\,(\frac{d}{dr}\mathrm{R}(r)) + r^2\,(\frac{d^2}{dr^2}\mathrm{R}(r)))}{\mu\,r^2} + \frac{1}{2}\frac{l\,(l+1)\,h_^2\,\mathrm{R}(r)}{\mu\,r^2} = En\,\mathrm{R}(r)$$

```
> Soln1 := dsolve(Eq1, R(r));
```

$$Soln1 := \mathrm{R}(r) = \frac{_C1\ \mathrm{BesselJ}\left(l+\frac{1}{2},\ \frac{\sqrt{2}\,\sqrt{En\,\mu}\,r}{h_}\right)}{\sqrt{r}} + \frac{_C2\ \mathrm{BesselY}\left(l+\frac{1}{2},\ \frac{\sqrt{2}\,\sqrt{En\,\mu}\,r}{h_}\right)}{\sqrt{r}}$$

The solution of the radial equation is a combination of Bessel functions. Because our region of interest includes $r = 0$, we choose the Bessel function of the first kind $J_\nu(x)$, or in Maple `BesselJ`, which we discuss extensively in Section 5.5. The solution of the radial equation is then

$$R(r) = \frac{C_1}{\sqrt{r}}J_{l+1/2}\left(\frac{\sqrt{2\mu E}}{\hbar}r\right). \tag{16.63}$$

There exists a definition of the spherical Bessel function,

$$j_l(\rho) = \left(\frac{\pi}{2\rho}\right)^{1/2}J_{l+1/2}(\rho); \tag{16.64}$$

adopting this definition, we find that the radial function $R(r)$ is simply the spherical Bessel function. Although one can express spherical Bessel functions as sinusoidal functions, such as

$$j_0(\rho) = \frac{\sin\rho}{\rho},$$

$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho},$$

$$j_2(\rho) = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin\rho - \frac{3}{\rho^2}\cos\rho, \tag{16.65}$$

we employ the original Bessel functions instead of using spherical Bessel functions; our treatment hence remains consistent with that in preceding chapters.

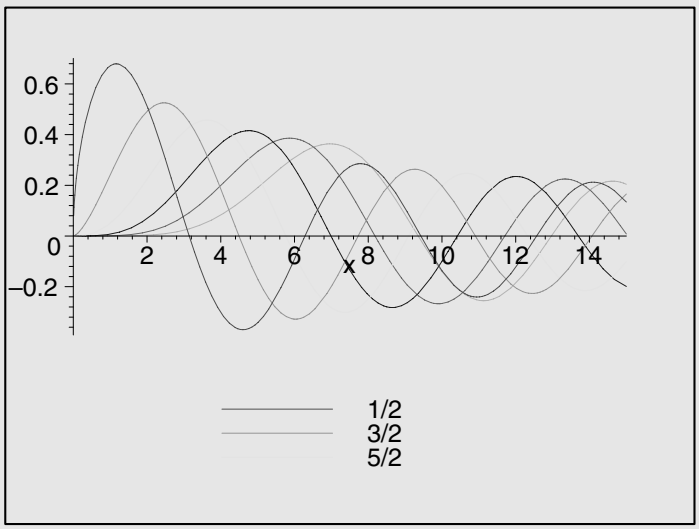
Because the potential energy is infinite for $r > a$, to ensure continuity of the wave function at the boundary, $R(a)$ must there be zero; that is,

$$J_{l+1/2}\left(\frac{\sqrt{2\mu E}}{\hbar}a\right) = 0. \tag{16.66}$$

This condition produces quantization of energy; to calculate its discrete values, we evaluate the zeros of the Bessel functions for a given value of l. Maple is capable of this task.

Worksheet 16.9 It is a simple task to use the `fsolve` command to find numerical values of roots of the Bessel functions. We make a diagram of the magnitudes of the square of these roots, which are proportional to the energy levels.

```
> plot([BesselJ(1/2, x), BesselJ(3/2, x), BesselJ(5/2, x),
> BesselJ(7/2, x), BesselJ(9/2, x), BesselJ(11/2, x)], x=0..15,
> legend=["1/2", "3/2", "5/2", "7/2", "9/2", "11/2"]);
```




```
> r[1] := fsolve(BesselJ(1/2, x), x=3..4);
```

$$r_1 := 3.141592654$$

```
> r[2] := fsolve(BesselJ(1/2, x), x=6..7);
```

$$r_2 := 6.283185307$$

```
> r[3] := fsolve(BesselJ(1/2, x), x=9..10);
```
$$r_3 := 9.424777961$$

```
> r[4] := fsolve(BesselJ(1/2, x), x=12..13);
```
$$r_4 := 12.56637061$$

```
> r[5] := fsolve(BesselJ(3/2, x), x=4..5);
```
$$r_5 := 4.493409458$$

```
> r[6] := fsolve(BesselJ(3/2, x), x=7..8);
```
$$r_6 := 7.725251837$$

```
> r[7] := fsolve(BesselJ(3/2, x), x=10..11);
```
$$r_7 := 10.90412166$$

```
> r[8] := fsolve(BesselJ(5/2, x), x=5..6);
```
$$r_8 := 5.763459197$$

```
> r[9] := fsolve(BesselJ(5/2, x), x=9..10);
```
$$r_9 := 9.095011330$$

```
> r[10] := fsolve(BesselJ(5/2, x), x=12..13);
```
$$r_{10} := 12.32294097$$

```
> r[11] := fsolve(BesselJ(7/2, x), x=6..7);
```
$$r_{11} := 6.987932001$$

```
> r[12] := fsolve(BesselJ(7/2, x), x=10..11);
```
$$r_{12} := 10.41711855$$

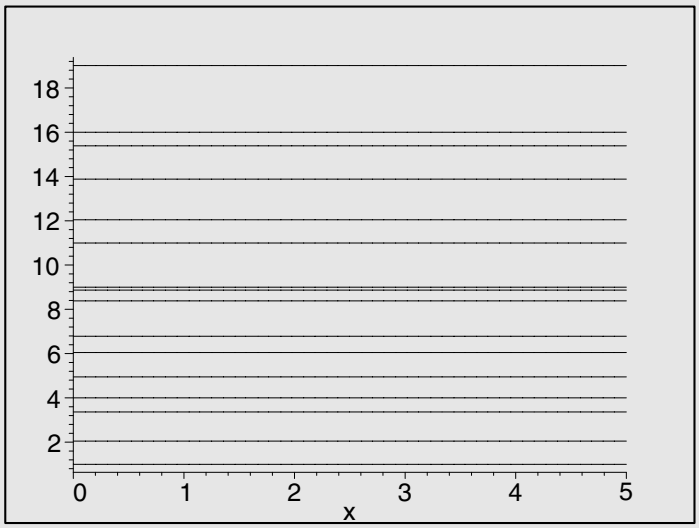
```
> r[13] := fsolve(BesselJ(7/2, x), x=13..14);
```
$$r_{13} := 13.69802315$$

```
> r[14] := fsolve(BesselJ(9/2, x), x=8..9);
```
$$r_{14} := 8.182561453$$

```
> r[15] := fsolve(BesselJ(9/2, x), x=11..12);
```
$$r_{15} := 11.70490715$$

```
> r[16] := fsolve(BesselJ(11/2, x), x=9..10);
```
$$r_{16} := 9.355812111$$

```
> plot({seq((r[i]/Pi)^2, i=1..16)}, x=0..5);
```



From the plots of those Bessel functions and their numerical solutions, we tabulate the roots of $J_{l+1/2}(x)$:

$$J_{l+1/2}(x_{ln}) = 0, \quad n = 1, 2, 3, \ldots, \tag{16.67}$$

where x_{ln} is the nth root of $J_{l+1/2}(x)$.

$$\begin{array}{ll} l = 0, & x_{0n} = 3.14, 6.28, 9.42, 12.57, \ldots \\ l = 1, & x_{1n} = 4.49, 7.73, 10.90, \ldots \\ l = 2, & x_{2n} = 5.76, 9.10, 12.32, \ldots \\ l = 3, & x_{3n} = 6.99, 10.42, 13.70, \ldots \\ l = 4, & x_{4n} = 8.18, 11.70, \ldots \\ l = 5, & x_{4n} = 9.36, \ldots \end{array} \tag{16.68}$$

The discrete energies are found as

$$\frac{\sqrt{2\mu E_{ln}}}{\hbar} a = x_{ln}, \quad E_{ln} = x_{ln}^2 \frac{\hbar^2}{2\mu a^2}. \tag{16.69}$$

We compare this infinite spherical well with the one-dimensional infinite well, of which the energies of the discrete states are

$$E_n = n^2 \pi^2 \frac{\hbar^2}{2\mu a^2}. \tag{16.70}$$

In the one-dimensional case, the solution of the Schrödinger equation is the sine function; the roots are therefore $n\pi$. In the three-dimensional case, we replace $n\pi$ by x_{ln}.

Table 16.4: Energy levels for the infinite spherical well.

l	n	Notation	$E_{ln}/[\hbar^2/(2\mu a^2)]$
0	1	$1s$	3.14
1	1	$1p$	4.49
2	1	$1d$	5.76
0	2	$2s$	6.28
3	1	$1f$	6.99
1	2	$2p$	7.73
4	1	$1g$	8.18
2	2	$2d$	9.10
5	1	$1h$	9.36
0	3	$3s$	9.42

The complete wave function (unnormalized) for an infinite spherical well is

$$\psi_{lmn} = \frac{1}{\sqrt{r}} J_{l+1/2}\left(x_{ln}\frac{r}{a}\right) Y_{lm}(\theta,\phi). \tag{16.71}$$

We label the states according to notation similar to that in the preceding section, with an important difference: the index n is *not* the principal quantum number, but simply the nth root of the Bessel function, in accordance with the discussion in Section 5.5. We sort the energies in increasing order in Table 16.4.

An atomic nucleus is characterized by the number of protons Z (atomic number) and the number of neutrons N that it contains. Some nuclei with particular values of Z and/or N show particular stability relative to their neighboring species; these values of Z and N are known as magic numbers and are experimentally observed to be

$$Z \text{ and/or } N = 2, 8, 20, 28, 50, 82, 126. \tag{16.72}$$

The situation is analogous to the characteristic stability of noble gases, for which

$$Z = 2, 10, 18, 36, 54, 86. \tag{16.73}$$

Unlike atomic physics, in which we understand the interaction between two charged particles, namely the Coulomb force, the interactions among protons and neutrons are incompletely characterized. The infinite spherical well serves as a crude approximation for a potential in nuclear physics that can explain the first three magic numbers. A nucleon is a fermion: thus it obeys Pauli's exclusion principle. To generate magic numbers at values 2, 8, 20, 34 and so on, requires that a $1s$ state can hold 2 nucleons, and a $1p$ state can hold 6; $1d$ and $2s$ have similar energies, and together they can hold $10 + 2 = 12$ nucleons; the $1f$ state can hold 14 nucleons. Although this crude model becomes incorrect in the fourth number, having even the first three magic numbers correct is encouraging!

It is understandable that an infinite spherical well is unrealistic; to improve this model one must choose a more suitable potential. This situation is similar to calculations for a self-

Table 16.5: Nuclear energy levels.

$1s_{1/2}$	2
$1p_{3/2}$, $1p_{1/2}$	6
$1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$	12
$1f_{7/2}$	8
$2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$, $1g_{9/2}$	22
$2d_{5/2}$, $1g_{7/2}$, $1h_{11/2}$, $2d_{3/2}$, $3s_{1/2}$	32
$2f_{7/2}$, $1h_{9/2}$, $1i_{13/2}$, $2f_{5/2}$, $3p_{3/2}$, $3p_{1/2}$	44

consistent potential $V(r)$ that yields an orbital energy associated with $3d$ less than that associated with $4s$. If we use the Coulomb potential which produces no crossing of $3d$ and $4s$, we predict stable elements to occur at $Z = 2$, 10, 28, 60, ..., according to which we might expect nickel to be a noble gas. Furthermore, one must include the nuclear spin-orbital potential to obtain proper magic numbers; in brief, the energy level depends on the orientation of the nuclear spin relative to its angular momentum. Because a nucleon has spin $\frac{1}{2}$, the total angular momentum of a nucleon is $j = l \pm \frac{1}{2}$. In additional to n and l, the energy depends strongly on j; the states are denoted by symbols $1s_{1/2}$, $1p_{1/2}$, etc., where the suffix specifies the value of j. The nuclear spin-orbital potential leads to large splittings of the energy, and the gap between $1f_{7/2}$ and $1f_{5/2}$ is responsible for the magic number 28. Similar to the grouping for the atomic energy levels, the nuclear energy levels are grouped as in Table 16.5. This work was done in 1949 by Maria Göppert-Mayer and independently by J. H. D. Jensen and his collaborators.

Exercises

1. For equation (16.5),

$$-\frac{\hbar^2}{2\mu r^2}\frac{d}{dr}\left[r^2\frac{dR(r)}{dr}\right] + \left[\frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)\right]R(r) = ER(r),$$

   let us define

$$R(r) = \frac{u(r)}{r}, \tag{16.74}$$

   prove that the radial equation for a three-dimensional central-force problem is reduced to an equivalent one-dimensional problem:

$$\frac{d^2u}{dr^2} + \left\{\frac{2\mu}{\hbar^2}[E - V(r)] - \frac{l(l+1)}{r^2}\right\}u = 0. \tag{16.75}$$

2. Using equation (16.34), make the change of variable to derive equation (16.33).

   Hint: the `dchange` command in the `PDEtools` package might be useful.

3. The average radius of a hydrogen atom is

$$\overline{r_{nl}} = n^2 a_0 \left\{ 1 + \frac{1}{2} \left[1 - \frac{l(l+1)}{n^2} \right] \right\}. \tag{16.76}$$

Verify this formula for all quantum states of the hydrogen atom for which $n = 3$ and $n = 4$ ($3s$, $3p$, $3d$, $4s$, $4p$, $4d$ and $4f$). To perform this task, evaluate an integral

$$\overline{r_{nl}} = \int_0^\infty r |R_{nl}|^2 r^2 dr. \tag{16.77}$$

Remember that r^2 arises from the volume element in spherical coordinates.

4. In an atom, an electron experiences a force deviating from Coulomb's law because of shielding. Consider an electron to be influenced by a Coulomb potential with an r^{-2} addition:

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r} + b\frac{1}{r^2}. \tag{16.78}$$

A potential function of this form, referred to as the Kratzer potential, can be exactly solved. Prove that discrete energies for this system conform to the formula

$$E_{n_r,l} = -\frac{1}{\left[n_r + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 + \frac{8\pi^2\mu b}{h^2}} \right]^2} \frac{\mu e^4}{8h^2\epsilon_0^2}. \tag{16.79}$$

For small b, expand the expression

$$\sqrt{\left(l + \frac{1}{2}\right)^2 + \frac{8\pi^2\mu b}{h^2}}$$

about $b = 0$, so to express the energy as

$$E_{n,l} = -\frac{1}{(n + \Delta_l)^2} \frac{\mu e^4}{8h^2\epsilon_0^2}, \tag{16.80}$$

where $n = n_r + l + 1$, as in the hydrogen atom. The term Δ_l is sometimes known as the Rydberg correction; express it in terms of b, l, μ and h.

Hints: one can exactly follow Section 16.4, but replace $l(l+1)$ with $s(s+1) \equiv l(l+1) + 8\pi^2\mu b/h^2$; alternatively, see Appendix B.2.3, and apply the same argument to obtain the discrete energies.

5. Unfortunately, the approach in the preceding problem is unsatisfactory for shielding in atomic physics, but the mathematics is almost identical for the relativistic Schrödinger equation, commonly referred to as the Klein–Gordon equation.

(a) For a differential equation

$$\frac{d^2u}{dr^2} + \left(-A + \frac{B}{r} + \frac{C}{r^2}\right) u = 0, \tag{16.81}$$

prove that the condition for u to be finite everywhere is

$$\frac{1}{2} + \frac{1-4C}{2} - \frac{B}{2\sqrt{A}} = -n_r, \tag{16.82}$$

where n_r is a positive integer.

(b) With the Coulomb potential, the radial part of the Klein–Gordon equation becomes[7]

$$\frac{d^2u}{dr^2} + \left\{\frac{1}{\hbar^2c^2}\left[\left(E + \frac{Ze^2}{r}\right)^2 - m^2c^4\right] - \frac{l(l+1)}{r^2}\right\} u = 0. \tag{16.83}$$

From the differential equation we just solved, identify that

$$A = \frac{m^2c^4 - E^2}{\hbar^2c^2}, \quad B = \frac{2EZ\alpha}{\hbar c}, \quad C = Z^2\alpha^2 - l(l+1),$$

where the fine-structure constant is

$$\alpha \equiv \frac{e^2}{\hbar c} \simeq \frac{1}{137}. \tag{16.84}$$

(In this problem we use the Gaussian system of units, and m stands for mass, not magnetic quantum number.) Thus, the discrete energy levels are

$$E = mc^2 \left\{1 + \frac{Z^2\alpha^2}{\left[n_r + \sqrt{\left(l+\frac{1}{2}\right)^2 - Z^2\alpha^2} + \frac{1}{2}\right]^2}\right\}^{1/2}. \tag{16.85}$$

(c) Expand the energy in a series of powers of α, and use the definition of the principal quantum number as $n = n_r + l + 1$, show that

$$E = mc^2\left[1 - \frac{Z^2\alpha^2}{2n^2} - \frac{Z^4\alpha^4}{2n^4}\left(\frac{n}{l+1/2} - \frac{3}{4}\right) + \ldots\right]. \tag{16.86}$$

6. The matrix element of an electric dipole moment for a transition taken between initial and final states is defined as

$$p_{fi} \equiv \left| \int \psi_f^* \, e\mathbf{r} \, \psi_i \, d\tau \right|. \tag{16.87}$$

[7] S. Weinberg, *The Quantum Theory of Fields*, Cambridge; New York: Cambridge University Press, 1995, vol. 1, p. 5.

With regard to the wave functions of atomic hydrogen, the matrix element of the electric dipole moment between $3d$ and $2p$ states is

$$p_{fi} = e \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \int_0^{\infty} dr \left(r^2 \psi^*_{210}\, r\, \psi_{320} \right). \tag{16.88}$$

To evaluate the integral explicitly, we split it into a radial part and an angular part.

(a) For the radial part, evaluate this integral,

$$\int_0^{\infty} R_{21} R_{32}\, r^3\, dr,$$

where R_{nl} is the radial part of the wave function listed in Table 16.2. The factor r^3 arises from the product of the volume element in spherical coordinates, r^2, and the electric dipole moment, r.

(b) The angular part of the solution involves spherical harmonics, and the integrals yield a simple factor. For a general situation, choose a few sets of l and m, and verify that

$$I_z = \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)\, (Y^*_{l'm} \cos\theta Y_{lm}) \neq 0 \text{ only if } l' = l \pm 1, \tag{16.89}$$

$$I_x = \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)\, (Y^*_{l'm'} \sin\theta \cos\phi Y_{lm}) \neq 0$$
$$\text{only if } l' = l \pm 1 \text{ and } m' = m \pm 1, \tag{16.90}$$

$$I_y = \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)\, (Y^*_{l'm'} \sin\theta \sin\phi Y_{lm}) \neq 0$$
$$\text{only if } l' = l \pm 1 \text{ and } m' = m \pm 1. \tag{16.91}$$

These results justify the selection rules for an electric-dipole transition that $\Delta l = \pm 1$, and $\Delta m = 0, \pm 1$.

7. Calculate the electric potential due to an electron in the $m = \pm 1$ states of the $3p$ level in hydrogen.

8. The angular part of spherical harmonics $Y_{lm}(\theta, \phi)$ can be linearly combined using Euler's formula for $l = 2$; one can construct five functions as (neglecting a factor of $1/\sqrt{4\pi}$)

$$\begin{aligned}
d_{z^2} &= \sqrt{5/4}\,(3\cos^2\theta - 1), \\
d_{yz} &= \sqrt{15}\,\sin\theta\,\cos\theta\,\cos\phi, \\
d_{xz} &= \sqrt{15}\,\sin\theta\,\cos\theta\,\sin\phi, \\
d_{xy} &= \sqrt{15/4}\,\sin^2\theta\,\sin 2\phi, \\
d_{x^2+y^2} &= \sqrt{15/4}\,\sin^2\theta\,\cos 2\phi.
\end{aligned} \tag{16.92}$$

(a) Plot the angular dependence of the above five functions, analogous to those in the worksheets in Section 16.5; note that d_{z^2} is identical to $Y_{20}(\theta, \phi)$.

(b) A set of six equivalent octahedral orbitals, d^2sp^3, formed from two d orbitals, the s orbital, and the three p orbitals, is

$$o_1 = \frac{1}{\sqrt{6}}s + \frac{1}{\sqrt{2}}p_z + \frac{1}{\sqrt{3}}d_{z^2}, \tag{16.93a}$$

$$o_2 = \frac{1}{\sqrt{6}}s - \frac{1}{\sqrt{2}}p_z + \frac{1}{\sqrt{3}}d_{z^2}, \tag{16.93b}$$

$$o_3 = \frac{1}{\sqrt{6}}s + \frac{1}{\sqrt{2}}p_x - \frac{1}{\sqrt{12}}d_{z^2} + \frac{1}{2}d_{x^2+y^2}, \tag{16.93c}$$

$$o_4 = \frac{1}{\sqrt{6}}s - \frac{1}{\sqrt{2}}p_x - \frac{1}{\sqrt{12}}d_{z^2} + \frac{1}{2}d_{x^2+y^2}, \tag{16.93d}$$

$$o_5 = \frac{1}{\sqrt{6}}s + \frac{1}{\sqrt{2}}p_y - \frac{1}{\sqrt{12}}d_{z^2} - \frac{1}{2}d_{x^2+y^2}, \tag{16.93e}$$

$$o_6 = \frac{1}{\sqrt{6}}s - \frac{1}{\sqrt{2}}p_y - \frac{1}{\sqrt{12}}d_{z^2} - \frac{1}{2}d_{x^2+y^2}. \tag{16.93f}$$

Plot the angular dependence of these functions.

(c) A set of four orbitals directed to the corners of a square can be formed as

$$q_1 = \frac{1}{2}s + \frac{1}{\sqrt{2}}p_x + \frac{1}{2}d_{xy}, \tag{16.94a}$$

$$q_2 = \frac{1}{2}s - \frac{1}{\sqrt{2}}p_x + \frac{1}{2}d_{xy}, \tag{16.94b}$$

$$q_3 = \frac{1}{2}s + \frac{1}{\sqrt{2}}p_y - \frac{1}{2}d_{xy}, \tag{16.94c}$$

$$q_4 = \frac{1}{2}s - \frac{1}{\sqrt{2}}p_y - \frac{1}{2}d_{xy}, \tag{16.94d}$$

which are called the dsp^2 orbitals. Plot the angular dependence of these functions.

9. The power of Maple is not limited to the topics which we discuss in this book. Among many topics we are unable to cover in this volume, we intend that the reader recognize the utility of Maple for calculations relating to quantum mechanics with this problem. Two of the most important approximation methods in quantum mechanics are perturbation theory and the variational principle; the treatment of a helium atom offers an excellent example.[8]

[8]Landau and Lifshitz (*QM*) 1977, p. 260; J. J. Sakurai, *Modern Quantum Mechanics*, Reading, MA: Addison-Wesley, 1994, p. 367.

(a) The first-order perturbation for the helium atom is (in the Gaussian system of units)

$$4^2\left(\frac{Z}{a_0}\right)^6 e^2 \int_0^\infty \left[\int_0^{r_1} \frac{1}{r_1} e^{-(2Z/a_0)(r_1+r_2)} r_2^2\, dr_2 + \int_{r_1}^\infty \frac{1}{r_2} e^{-(2Z/a_0)(r_1+r_2)} r_2^2\, dr_2\right] r_1^2 dr_1; \quad (16.95)$$

evaluate this integral.

(b) Find the value of Z_{eff} that minimizes $\overline{H}$ in the following equation:

$$\overline{H} = Z_{\text{eff}}^2 - 2ZZ_{\text{eff}} + \frac{5}{8}Z_{\text{eff}}; \quad (16.96)$$

this calculation is encountered when applying the variational method for a helium atom.

Answer: (a) $\frac{5Ze^2}{8a_0}$; (b) $Z_{\text{eff}} = Z - \frac{5}{16}$.

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17 Quantum Statistics

The essence of statistical mechanics is to calculate macroscopic quantities by averaging over numerous microscopic states of constituent particles; many such calculations involve improper integrals. In some limiting conditions, such as extreme dilution or high temperature, Maple can perform the integrations to obtain exact results. In most other situations, such integrals admit no expression in closed form; we therefore introduce various expansion techniques to simplify the expressions.

17.1 Statistical Distributions

In an equilibrium system, suppose that one particular macroscopic state has energy E; the probability $P(E)$ that the system is found in this state among all possible states is

$$P(E) = \frac{e^{-\beta E}}{\sum_E e^{-\beta E}}; \tag{17.1}$$

the definition of β is

$$\beta = \frac{1}{kT}, \tag{17.2}$$

where k is the Boltzmann constant and T is the temperature. The sum in the denominator of equation (17.1), which runs over all possible states of energy E, is called the partition function Z,

$$Z = \sum_E e^{-\beta E}. \tag{17.3}$$

All thermodynamic functions such as the pressure, specific heat, and so forth, can be deduced from the partition function. Consider a system of N indistinguishable identical particles; as a first approximation, we treat them as an ideal gas, in which there is no interaction between particles. We denote the energy of an individual particle as ε, and the number of particles with this energy as n_ε. The energy of the entire system is

$$E = \sum_\varepsilon n_\varepsilon \varepsilon. \tag{17.4}$$

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We distinguish between ε, which denotes the energy of a single particle, and E, which denotes the energy of one state of the entire system.

For a closed system, the partition function Z is subject to the condition that

$$N = \sum_{\varepsilon} n_{\varepsilon}. \tag{17.5}$$

According to quantum mechanics, the values permitted for n_ε are related to the intrinsic angular momentum of the particles – spin. Particles of integer spin, or bosons, obey the Bose–Einstein statistics; particles of half-integer spin, or fermions, obey the Fermi–Dirac statistics. A restriction for particles of these two classes is that for

- Bose–Einstein statistics: $n_\varepsilon = 0, 1, 2, 3, \ldots$;
- Fermi–Dirac statistics: $n_\varepsilon = 0, 1$.

Instead of using the partition function directly, we use the mean value of n_ε, denoted $\overline{n}_\varepsilon$, to describe the system. The mean occupation number can be calculated from the partition function:

$$\overline{n}_\varepsilon = \frac{\sum_E n_\varepsilon e^{-\beta(n_1\varepsilon_1+n_2\varepsilon_2+\ldots)}}{\sum_E e^{-\beta(n_1\varepsilon_1+n_2\varepsilon_2+\ldots)}} = \frac{1}{Z}\sum_E \left(-\frac{1}{\beta}\frac{\partial}{\partial\varepsilon}\right) e^{-\beta\sum_\varepsilon n_\varepsilon\varepsilon} = -\frac{1}{\beta Z}\frac{\partial Z}{\partial\varepsilon}, \tag{17.6}$$

or

$$\overline{n}_\varepsilon = -\frac{1}{\beta}\frac{\partial \ln Z}{\partial\varepsilon}. \tag{17.7}$$

Evaluating the partition function with the restriction on the number of particles given by equation (17.5) is complicated, but by introducing a chemical potential μ, the energy required to remove a particle from the system, accommodates this restriction. Omitting the derivation, we list the results for mean occupation numbers for these two statistics:

- Bose–Einstein statistics

$$\boxed{\overline{n}_\varepsilon = \frac{1}{e^{\beta(\varepsilon-\mu)}-1}}; \tag{17.8}$$

- Fermi–Dirac statistics

$$\boxed{\overline{n}_\varepsilon = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}}. \tag{17.9}$$

As each mean occupation number indicates the distribution of particles over various quantum states, each of them is commonly called a distribution. They constitute the most useful information in statistical mechanics: we can calculate any thermodynamic function from these distributions.

Because we treat energy levels ε near to each other, we replace the sum over states by an integral in the phase space:

$$g\, d^3x\, d^3p \rightarrow \frac{gV}{h^3}\, d^3p.$$

In this expression, g is the number of possible spin orientations of the particle. Because the integrand is independent of position, we integrate d^3x to obtain the volume V. Because of the uncertainty principle $dx \times dp \cong h$, we divide the phase space into basic cells each of volume h^3.

Two obvious quantities that we can directly calculate are N and E. Replacing the sum in equation (17.5) by an integral, we write the number of particles as

$$N = \frac{gV}{h^3} \int_0^\infty \overline{n}_\varepsilon d^3p. \tag{17.10}$$

We, analogously, calculate the internal energy U, which is the average of the energy $\overline{E}$,

$$U = \overline{E} = \frac{gV}{h^3} \int_0^\infty \varepsilon \overline{n}_\varepsilon d^3p. \tag{17.11}$$

Any other thermodynamic function comes out of an appropriate calculation; in this chapter, we concentrate on the pressure P and the specific heat C_V. Both pressure and specific heat are closely related to the internal energy. The pressure is obtained from

$$P = \frac{g}{h^3} \int_0^\infty \left(\frac{p}{3} \frac{d\varepsilon}{dp} \right) \overline{n}_\varepsilon d^3p. \tag{17.12}$$

This equation essentially indicates that the pressure is one third of the particle density multiplied by the average of the product of the momentum and the velocity, a result well known in gas kinematics; the reader can consult relevant literature for a derivation.[1] Take care to distinguish between the symbol P for pressure and p for momentum. For ε of a given form, the pressure differs from the energy density by a factor, which we will show in subsequent sections.

The specific heat, which measures the capacity of a system to absorb thermal energy, is the derivative of the internal energy with respect to the temperature,

$$C_V = \left(\frac{\partial U}{\partial T} \right)_{N,V}, \tag{17.13}$$

here for constant volume and for a constant number of particles.

[1] Pathria 1996, p. 137ff.

17.2 Maxwell–Boltzmann Statistics

We begin our discussion by considering particles in a condition of low density. If the occupation number is much smaller than unity, that is,

$$(\varepsilon - \mu) \gg kT, \quad e^{\beta(\varepsilon-\mu)} \gg 1,$$

both Bose–Einstein and Fermi–Dirac statistics reduce to

$$\overline{n}_\varepsilon = e^{-\beta(\varepsilon-\mu)}. \tag{17.14}$$

This distribution pertains to Maxwell–Boltzmann statistics, which is the classical limit. We have already applied this distribution to paramagnetism in Section 13.5. In the plot below we compare these three types of statistics.

Worksheet 17.1 We define a parameter $\eta = \beta(\varepsilon - \mu)$ to plot these statistical distributions.

```
> ncl := 1/exp(eta);
```

$$ncl := \frac{1}{e^{\eta}}$$

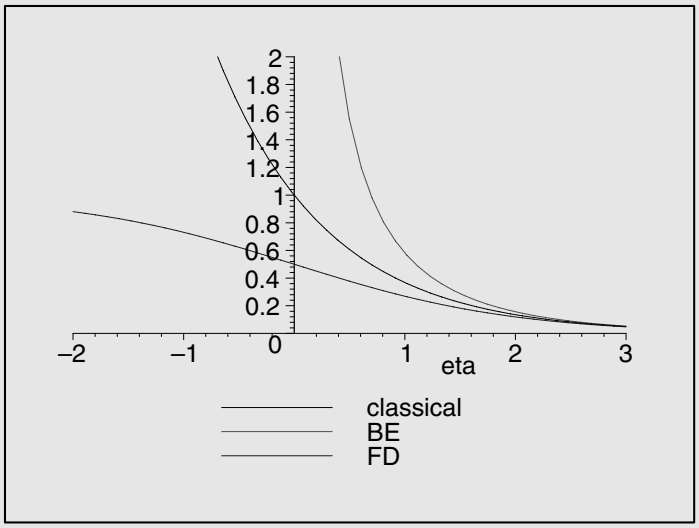
```
> nbe := 1/(exp(eta) - 1);
```

$$nbe := \frac{1}{e^{\eta} - 1}$$

```
> nfd := 1/(exp(eta) + 1);
```

$$nfd := \frac{1}{e^{\eta} + 1}$$

```
> plot([ncl, nbe, nfd], eta=-2..3, 0..2, legend=["classical", "BE",
> "FD"]);
```



This plot makes clear that Maxwell–Boltzmann statistics is a satisfactory approximation at low density, for which $\eta \gg 1$.

For other than the era of the early universe, or a situation one might encounter in a high-energy research laboratory, it suffices to express the kinetic energy in the nonrelativistic form,

$$\varepsilon = \frac{p^2}{2m}. \tag{17.15}$$

We calculate the element of momentum space as

$$d^3p = 4\pi p^2 dp = 4\sqrt{2}\pi m^{3/2}\varepsilon^{1/2}d\varepsilon, \quad (p = \sqrt{2m\varepsilon}).$$

The element of the phase space is therefore

$$\frac{V}{h^3}d^3p = \frac{V}{h^3}4\sqrt{2}\pi m^{3/2}\varepsilon^{1/2}d\varepsilon. \tag{17.16}$$

We introduce the fugacity, defined as

$$z \equiv e^{\beta\mu}; \tag{17.17}$$

this quantity regularly appears in subsequent sections.

Using the distribution for Maxwell–Boltzmann statistics, we calculate the number of particles:

$$N = \frac{V}{h^3}\int_0^\infty ze^{-\varepsilon/kT}4\sqrt{2}\pi m^{3/2}\varepsilon^{1/2}d\varepsilon = \frac{Vz}{h^3}(2\pi mkT)^{3/2}. \tag{17.18}$$

We have mentioned in the preceding section that the chemical potential μ regulates the number of particles N. In most experiments, we measure T, the number of particles N, and the volume V; the ratio of the latter two is the number density n,

$$n = \frac{N}{V}. \tag{17.19}$$

From a given n, we can derive μ. We seek to express thermodynamic functions in terms of N, V and T; for this purpose we need to solve for z and then for the chemical potential μ in terms of N, V and T:

$$z = \frac{N}{V}\left(\frac{h}{2\pi mkT}\right)^{3/2}, \quad \mu = kT\ln z = kT\ln\left[\frac{N}{V}\left(\frac{h^2}{2\pi mkT}\right)^{3/2}\right]. \tag{17.20}$$

The internal energy is

$$U = \frac{V}{h^3}\int_0^\infty ze^{-\varepsilon/kT}4\sqrt{2}\pi m^{3/2}\varepsilon^{3/2}d\varepsilon = \frac{3}{2}kT\frac{Vz}{h^3}(2\pi mkT)^{3/2}; \tag{17.21}$$

eliminating z from this expression yields

$$U = \frac{3}{2}NkT. \tag{17.22}$$

We find the derivative in equation (17.12) from given ε in equation (17.15),

$$\frac{p}{3}\frac{d\varepsilon}{dp} = \frac{2}{3}\varepsilon.$$

We conclude accordingly that under nonrelativistic conditions, the pressure is two-thirds of the energy density:

$$P = \frac{2}{3}\frac{U}{V} = \frac{NkT}{V}. \tag{17.23}$$

This relation is the familiar equation of state of a classical ideal gas.

The specific heat is

$$C_V = \left(\frac{\partial U}{\partial T}\right)_{N,V} = \frac{3}{2}Nk. \tag{17.24}$$

We have therefore shown that quantum statistics under a condition of low density yields the well-known thermodynamic relations of a classical ideal gas.

Worksheet 17.2 The symbols `ncl` and `Epr1` signify the Maxwell–Boltzmann distribution and the element of the momentum space, respectively. All the integrals are evaluated directly. We solve for z from the equation of N, then obtain the chemical potential μ. We express the energy and pressure in terms of N, V and T by eliminating z.

```
> assume(k>0, T>0, m>0);
> ncl := 1/(exp(epsilon/(k*T))/z);
```

$$ncl := \frac{z}{e^{(\frac{\varepsilon}{kT})}}$$

```
> p := sqrt(2*m*epsilon);
```

$$p := \sqrt{2}\sqrt{m\,\varepsilon}$$

```
> Epr1 := 4*Pi*p^2*diff(p, epsilon);
```

$$Epr1 := \frac{4\,\pi\,m^2\,\varepsilon\,\sqrt{2}}{\sqrt{m\,\varepsilon}}$$

```
> Eq2 := N = V/(h^3)*int(ncl*Epr1, epsilon=0..infinity);
```

$$Eq2 := N = \frac{2\,V\,z\,\pi^{(3/2)}\,m^{(3/2)}\,\sqrt{2}}{h^3\left(\frac{1}{k\,T}\right)^{(3/2)}}$$

```
> Eq3 := En =V/(h^3)*int(ncl*epsilon*Epr1, epsilon=0..infinity);
```

$$Eq3 := En = \frac{3\,V\,z\,\pi^{(3/2)}\,m^{(3/2)}\,\sqrt{2}}{h^3\left(\frac{1}{k\,T}\right)^{(5/2)}}$$

```
> Eq4 := isolate(Eq2, z);
```

$$Eq4 := z = \frac{N\,h^3\,\sqrt{2}\,\left(\frac{1}{k\,T}\right)^{(3/2)}}{4\,V\,\pi^{(3/2)}\,m^{(3/2)}}$$

```
> Eq5 := mu = k*T*ln(rhs(Eq4));
```

$$Eq5 := \mu = k\,T\ln\left(\frac{N\,h^3\,\sqrt{2}\,\left(\frac{1}{k\,T}\right)^{(3/2)}}{4\,V\,\pi^{(3/2)}\,m^{(3/2)}}\right)$$

```
> Eq6 := subs(Eq4, Eq3);
```

$$Eq6 := En = \frac{3\,N\,k\,T}{2}$$

```
> Eq7 := P = 2/3*rhs(Eq6)/V;
```

$$Eq7 := P = \frac{N\,k\,T}{V}$$

```
> Eq8 := C[V] = diff(rhs(Eq6), T);
```

$$Eq8 := C_V = \frac{3\,N\,k}{2}$$

17.3 Ideal Bose Gas

In the preceding section, we consider an approximate situation for which the density of particles is low, so that integrals can be evaluated exactly; in general, most integrals yield no analytic expression. We proceed to discuss the ideal Bose system. The distribution for Bose–Einstein statistics is

$$\overline{n}_\varepsilon = \frac{1}{e^{\beta(\varepsilon-\mu)}-1}. \tag{17.25}$$

To avoid a singularity of $\overline{n}_\varepsilon$ at $\varepsilon = \mu$, we must have μ less than every energy ε. For the nonrelativistic kinetic energy, the lowest value of ε is 0; therefore μ must be negative. Assuming $g = 1$, we neglect the factor for spin structure. The element of phase space is the same as in equation (17.16),

$$\frac{V}{h^3}d^3p = \frac{V}{h^3}4\sqrt{2}\pi m^{3/2}\varepsilon^{1/2}d\varepsilon.$$

Thus, the number of particles is

$$N = \frac{V}{h^3}\int_0^\infty \frac{4\sqrt{2}\pi m^{3/2}\varepsilon^{1/2}}{e^{\beta(\varepsilon-\mu)}-1}d\varepsilon, \tag{17.26}$$

and the internal energy is

$$U = \frac{V}{h^3} \int_0^\infty \frac{4\sqrt{2}\pi m^{3/2} \varepsilon^{3/2}}{e^{\beta(\varepsilon - \mu)} - 1} d\varepsilon. \tag{17.27}$$

To simplify the notation, we introduce parameters to abbreviate commonly appearing expressions. We define the mean thermal wavelength λ of particles to be

$$\lambda \equiv \frac{h}{\sqrt{2\pi m k T}}, \tag{17.28}$$

and a parameters x,

$$x \equiv \beta\varepsilon. \tag{17.29}$$

Recall the fugacity defined in the preceding section,

$$z \equiv e^{\beta\mu}. \tag{17.17}$$

We further define the Bose–Einstein integral function:

$$g_\sigma(z) = \frac{1}{\Gamma(\sigma)} \int_0^\infty \frac{x^{\sigma-1}}{z^{-1}e^x - 1}\, dx, \tag{17.30}$$

where $\Gamma(\sigma)$ is the gamma function, defined as

$$\Gamma(\sigma) \equiv \int_0^\infty t^{\sigma-1} e^{-t}\, dt, \quad \sigma > 0, \tag{17.31}$$

which is implemented in Maple.

With these definitions, we write

$$N = \frac{V}{\lambda^3} g_{3/2}(z), \tag{17.32}$$

and

$$U = \frac{3}{2} kT \frac{V}{\lambda^3} g_{5/2}(z). \tag{17.33}$$

Because U is an extensive quantity and is thus proportional to N, it is preferable to write U as

$$U = \frac{3}{2} NkT \frac{g_{5/2}(z)}{g_{3/2}(z)}. \tag{17.34}$$

In a nonrelativistic situation, the pressure is two-thirds of the energy density; hence

$$P = \frac{NkT}{V} \frac{g_{5/2}(z)}{g_{3/2}(z)}. \tag{17.35}$$

The specific heat results from differentiating the energy with respect to the temperature:

$$C_V = \left(\frac{\partial U}{\partial T}\right)_{N,V}. \tag{17.36}$$

There is no analytic form for these integrals, but Maple can numerically evaluate $g_\sigma(z)$ for any given σ and z. Although the above integrals express all quantities as a function of z, we generally do not know z, which is related to the chemical potential μ; instead we know N, V and T. In Maxwell–Boltzmann statistics, we solve for z explicitly in terms of N, V and T, but it is not feasible for other types of statistics. Nevertheless, using Maple we proceed to solve for z using the graphical method.

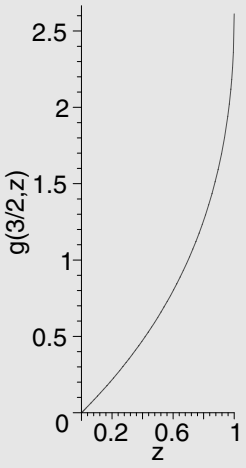
For Bose–Einstein statistics, because μ is negative, the possible range of z is $0 < z < 1$. We make a plot of $g_{3/2}(z)$ in this range.

Worksheet 17.3 In our definition of $g_\sigma(z)$, we invoke the gamma function, known as `GAMMA` in Maple. Although there is no analytic expression for the integral, we can produce a plot.

```
> g := (sigma, z) -> int(x^(sigma-1)/(exp(x)/z - 1),
> x=0..infinity)/GAMMA(sigma);
```

$$g := (\sigma,\, z) \to \frac{1}{\Gamma(\sigma)} \int_0^\infty \frac{x^{(\sigma-1)}}{\frac{e^x}{z} - 1}\, dx$$

```
> plot(g(3/2,z), z=0..1, scaling=constrained);
```




```
> g(3/2,1) = evalf(g(3/2,1));
```

$$\zeta\left(\frac{3}{2}\right) = 2.612375349$$

We write equation (17.32) as

$$n\lambda^3 = g_{3/2}(z). \tag{17.32$'$}$$

Our objective is to calculate the inverse function $g_{3/2}^{-1}$ so that we find z as

$$z = g_{3/2}^{-1}(n\lambda^3).$$

In the graph the horizontal axis is z and the vertical axis is $n\lambda^3$; we simply interchange axes so that numerically, for a given value of $n\lambda^3$, we find a corresponding z. An example of liquid ^{4}He appears in an exercise.

The condition at the classical limit is alternatively expressed as

$$n\lambda^3 \ll 1.$$

According to the graph, for small $n\lambda^3$, the function appears linear, that is $n\lambda^3 = g_{3/2}(z) \cong z$ for $z \ll 1$. This linear relation enables us to explicitly solve for z in the classical limit. When $n\lambda^3$ is of order unity, it departs significantly from the linear relation. We discuss the technique of virial expansion for $n\lambda^3 < 1$ in Section 17.3.1.

Another limit is for $z \cong 1$. From the graph, $g_{3/2}(1)$ is finite; more precisely,

$$g_{3/2}(1) = \zeta(3/2) = 2.612,$$

where $\zeta(\sigma)$ is the Riemann zeta function, defined as

$$\zeta(\sigma) = \sum_{l=1}^{\infty} \frac{1}{l^\sigma}. \tag{17.37}$$

This limit leads to the interpretation of the Bose–Einstein condensation, which we will discuss in Section 17.3.2.

17.3.1 Low Density and Virial Expansion

The context of what we call low density is the regime in which the classical limit is no longer adequate, but

$$n\lambda^3 < 1.$$

Under this condition, we modify the linear relation by adding terms of $n\lambda^3$ to the greater powers; our objective is to express all thermodynamic functions as a power series in $n\lambda^3$.

To express z as a power series of $n\lambda^3$, we first expand $g_{3/2}(z)$ in z so that equation (17.32$'$) becomes

$$n\lambda^3 = g_{3/2}(z) = z + \frac{z^2}{2^{3/2}} + \frac{z^3}{3^{3/2}} + \frac{z^4}{4^{3/2}} + \dots.$$

We then revert the power series to express z in terms of $n\lambda^3$. This process is made iterative until the precision is satisfactory. For the zeroth order we take only one term so that we can solve $z_0 = n\lambda^3$; for first order we take two terms and substitute z_0 for z. We proceed iteratively using the expression from a preceding approximation, illustrated as follows.

$$\begin{aligned}
&\mathcal{O}(0): \quad z_0 = n\lambda^3, \\
&\mathcal{O}(1): \quad z_1 = n\lambda^3 - \frac{z_0^2}{2^{3/2}}, \\
&\mathcal{O}(2): \quad z_2 = n\lambda^3 - \frac{z_1^2}{2^{3/2}} - \frac{z_1^3}{3^{3/2}}, \\
&\mathcal{O}(3): \quad z_3 = n\lambda^3 - \frac{z_2^2}{2^{3/2}} - \frac{z_2^3}{3^{3/2}} - \frac{z_2^3}{4^{3/2}}, \\
&\ldots.
\end{aligned}$$

This type of task is readily accomplished with Maple simply with the `solve` command; see the worksheet below. We have

$$z = n\lambda^3 - \frac{1}{2\sqrt{2}}(n\lambda^3)^2 + \left(\frac{1}{4} - \frac{1}{3\sqrt{3}}\right)(n\lambda^3)^3 + \ldots. \tag{17.38}$$

Knowing z in terms of $n\lambda^3$, we eliminate z from U and P, which are each a function of z in this form:

$$\frac{g_{5/2}(z)}{g_{3/2}(z)}.$$

We again expand both $g_{5/2}(z)$ and $g_{3/2}(z)$ in power series of z, substitute equation (17.38) for z, and make the expansion in $n\lambda^3$ to desired powers; U and P then can be expressed as

$$\frac{U}{N} = \frac{3}{2}kT\frac{g_{5/2}(z)}{g_{3/2}(z)} = \frac{3}{2}kT[1 + a_1(n\lambda^3) + a_2(n\lambda^3)^2 + a_3(n\lambda^3)^3 + \ldots], \tag{17.39}$$

and

$$P = \frac{1}{3}\frac{U}{V} = nkT\left[1 + a_1(n\lambda^3) + a_2(n\lambda^3)^2 + a_3(n\lambda^3)^3 + \ldots\right]. \tag{17.40}$$

An equation of state in this form is called the virial expansion, and a_1, a_2, ..., are virial coefficients.

Maple is particularly useful for performing this series expansion; we evaluate the virial coefficients to be

$$\begin{aligned}
&a_1 = -\tfrac{\sqrt{2}}{8} = -0.17678, \\
&a_2 = \tfrac{1}{8} - \tfrac{2\sqrt{3}}{27} = -0.0033, \\
&a_3 = -\tfrac{3}{32} - \tfrac{5\sqrt{2}}{64} + \tfrac{\sqrt{6}}{12} = -0.00011, \\
&\ldots.
\end{aligned} \tag{17.41}$$

The specific heat per particle is

$$\frac{C_V}{N} = \frac{1}{N}\left(\frac{\partial U}{\partial T}\right)_V . \tag{17.42}$$

According to the definition of mean thermal wavelength λ in equation (17.28),

$$\lambda \propto T^{-1/2};$$

so

$$\frac{C_V}{N} = \frac{3}{2}k[1 + 0.084n\lambda^3 + 0.0066(n\lambda^3)^2 + 0.0004(n\lambda^3)^3]. \tag{17.43}$$

Worksheet 17.4 We first define the integral $g_\sigma(z)$. Maple can expand $g_{3/2}(z)$ and $g_{5/2}(z)$ as a Taylor series, denoted `gee[3/2]` and `gee[5/2]`, respectively. To revert $g_{3/2}(z)$, we simply use the `solve` command; note that only for a series (not a polynomial) does `solve` effect a reversion. We use the symbol `A` for $n\lambda^3$. The ratio of $g_{5/2}(z)$ to $g_{3/2}(z)$ is assigned to `Epr1`, which is convenient for subsequent operations. To explicitly indicate the temperature dependence of λ in U, we substitute $K/\sqrt{T}$ for λ. After differentiating U with respect to T, we eliminate the constant of proportionality by substituting $\lambda\sqrt{T}$ for K.

```
> g := (sigma, z) -> int(x^(sigma-1)/(exp(x)/z - 1),
> x=0..infinity)/GAMMA(sigma);
```

$$g := (\sigma,\, z) \to \frac{1}{\Gamma(\sigma)} \int_0^\infty \frac{x^{(\sigma-1)}}{\frac{e^x}{z} - 1}\, dx$$

```
> gee[3/2] := taylor(g(3/2,z), z);
```

$$gee_{3/2} := z + \frac{\sqrt{2}}{4} z^2 + \frac{\sqrt{3}}{9} z^3 + \frac{\sqrt{4}}{16} z^4 + \frac{\sqrt{5}}{25} z^5 + \mathrm{O}(z^6)$$

```
> Soln1 := solve(A = gee[3/2], z);
```

$$Soln1 := A - \frac{\sqrt{2}}{4} A^2 + \left(\frac{1}{4} - \frac{\sqrt{3}}{9}\right) A^3 + \left(\frac{5\sqrt{2}\sqrt{3}}{36} - \frac{5\sqrt{2}}{32} - \frac{\sqrt{4}}{16}\right) A^4$$
$$+ \left(-\frac{\sqrt{5}}{25} + \frac{95}{288} - \frac{7\sqrt{3}}{24} + \frac{3\sqrt{4}\sqrt{2}}{32}\right) A^5 + \mathrm{O}(A^6)$$

```
> Eq3 := z = subs(A=n*lambda^3, convert(Soln1, polynom));
```

$$Eq3 := z = n\lambda^3 - \frac{\sqrt{2}\, n^2 \lambda^6}{4} + \left(\frac{1}{4} - \frac{\sqrt{3}}{9}\right) n^3 \lambda^9 + \left(\frac{5\sqrt{2}\sqrt{3}}{36} - \frac{5\sqrt{2}}{32} - \frac{\sqrt{4}}{16}\right) n^4 \lambda^{12}$$
$$+ \left(-\frac{\sqrt{5}}{25} + \frac{95}{288} - \frac{7\sqrt{3}}{24} + \frac{3\sqrt{4}\sqrt{2}}{32}\right) n^5 \lambda^{15}$$

```
> gee[5/2] := taylor(g(5/2, z), z);
```

$$gee_{5/2} := z + \frac{\sqrt{2}}{8} z^2 + \frac{\sqrt{3}}{27} z^3 + \frac{\sqrt{4}}{64} z^4 + \frac{\sqrt{5}}{125} z^5 + \mathrm{O}(z^6)$$

```
> Epr1 := convert(gee[5/2]/gee[3/2], polynom);
```

$$Epr1 := \frac{z + \frac{1}{8}\sqrt{2}\, z^2 + \frac{1}{27}\sqrt{3}\, z^3 + \frac{1}{64}\sqrt{4}\, z^4 + \frac{1}{125}\sqrt{5}\, z^5}{z + \frac{1}{4}\sqrt{2}\, z^2 + \frac{1}{9}\sqrt{3}\, z^3 + \frac{1}{16}\sqrt{4}\, z^4 + \frac{1}{25}\sqrt{5}\, z^5}$$

```
> Epr2 := subs(Eq3, Epr1):
```

```
> Epr3 := convert(taylor(Epr2, n, 5), polynom):
```

```
> Epr3 := collect(simplify(Epr3), n);
```

$$Epr3 := 1 + \left(-\frac{3}{32}\lambda^9 - \frac{5}{64}\lambda^9\sqrt{2} + \frac{1}{12}\lambda^9\sqrt{2}\sqrt{3}\right) n^3 + \left(\frac{1}{8}\lambda^6 - \frac{2}{27}\lambda^6\sqrt{3}\right) n^2 - \frac{\sqrt{2}\,\lambda^3 n}{8}$$

```
> Epr4 := evalf(Epr3);
```

$$Epr4 := 1. - 0.0001112893\, n^3 \lambda^9 - 0.0033000598\, n^2 \lambda^6 - 0.1767766952\, n\, \lambda^3$$

```
> Eq31 := P/(n*k*T) = Epr4;
```

$$Eq31 := \frac{P}{n\,k\,T} = 1. - 0.0001112893\, n^3 \lambda^9 - 0.0033000598\, n^2 \lambda^6 - 0.1767766952\, n\, \lambda^3$$

```
> Eq41 := U/N = 3*k*T/2*Epr4;
```

$$Eq41 := \frac{U}{N} = \frac{3\,k\,T\,(1. - 0.0001112893\, n^3 \lambda^9 - 0.0033000598\, n^2 \lambda^6 - 0.1767766952\, n\, \lambda^3)}{2}$$

```
> Eq42 := subs(lambda=K/sqrt(T), Eq41);
```

$$Eq42 := \frac{U}{N} = \frac{3\,k\,T\left(1. - \frac{0.0001112893\, n^3 K^9}{T^{(9/2)}} - \frac{0.0033000598\, n^2 K^6}{T^3} - \frac{0.1767766952\, n\, K^3}{T^{(3/2)}}\right)}{2}$$

```
> Eq43 := C[V]/N = diff(rhs(Eq42), T);
```

$$Eq43 := \frac{C_V}{N} = \frac{3\,k\left(1. - \frac{0.0001112893\,n^3\,K^9}{T^{(9/2)}} - \frac{0.0033000598\,n^2\,K^6}{T^3} - \frac{0.1767766952\,n\,K^3}{T^{(3/2)}}\right)}{2} + \frac{3\,k\,T\left(\frac{0.0005008018500\,n^3\,K^9}{T^{(11/2)}} + \frac{0.0099001794\,n^2\,K^6}{T^4} + \frac{0.2651650428\,n\,K^3}{T^{(5/2)}}\right)}{2}$$

```
> Eq44 := subs(K=lambda*sqrt(T), Eq43);
```

$$Eq44 := \frac{C_V}{N} = \frac{3\,k\left(1. - 0.0001112893\,n^3\,\lambda^9 - 0.0033000598\,n^2\,\lambda^6 - 0.1767766952\,n\,\lambda^3\right)}{2} + \frac{3\,k\,T\left(\frac{0.0005008018500\,n^3\,\lambda^9}{T} + \frac{0.0099001794\,n^2\,\lambda^6}{T} + \frac{0.2651650428\,n\,\lambda^3}{T}\right)}{2}$$

```
> Eq43 := collect(Eq44, n);
```

$$Eq43 := \frac{C_V}{N} = 0.0005842688250\,k\,\lambda^9\,n^3 + 0.009900179400\,k\,\lambda^6\,n^2 + 0.1325825214\,k\,\lambda^3\,n + 1.500000000\,k$$

17.3.2 Bose–Einstein Condensation at Low Temperature

Two values of the Riemann zeta function relevant in this section are

$$\zeta(3/2) = 2.612, \quad \zeta(5/2) = 1.341;$$

we obtain them from Maple by entering `Zeta(3/2)` and `Zeta(5/2)`.

The maximum allowed value of z for a system obeying Bose–Einstein statistics is unity. According to the graph of $n\lambda^3$ versus z, $g_{3/2}(z)$ converges to a finite number $\zeta(3/2) = 2.612$. Although our treatment seems to fail at high density for which $n\lambda^3 > 2.612$, this discrepancy is explicable. In all our calculations, we replace sums with integrals, for which the element of the phase space involves a factor $\varepsilon^{1/2}$. A consequence is that the quantum state of $\varepsilon = 0$ disappears from our counting. In normal circumstances, such an omission is negligible, but at low temperature it is significant.

To be more accurate, we should write equation (17.26) as

$$N - N_0 = \frac{V}{h^3}\int_0^\infty \frac{4\sqrt{2}\pi m^{3/2}\varepsilon^{1/2}}{e^{\beta(\mu-\varepsilon)}-1}d\varepsilon, \tag{17.44}$$

where N_0 is the number of particles in the state $\varepsilon = 0$ that is not counted in the integral. If we have a condition $n\lambda^3 > 2.612$, or explicitly with n and λ in their original definitions,

$$\frac{N}{V}\left(\frac{h}{\sqrt{2\pi mkT}}\right)^3 > \zeta(3/2),$$

we must have $N_0 > 0$ to accommodate the extra particles. There is theoretically no limit to the number of particles that can occupy the state with $\varepsilon = 0$. The phenomenon of Bose–Einstein condensation occurs when a great number of particles occupy the ground state, and the necessary condition for this condensation is

$$N > VT^{3/2}\frac{(2\pi mk)^{3/2}}{h^3}\zeta(3/2). \tag{17.45}$$

If we hold N and V constant and vary T, the condition for condensation becomes

$$T < T_c \equiv \frac{h^2}{2\pi mk}\left[\frac{1}{\zeta(3/2)}\frac{N}{V}\right]^{2/3}, \tag{17.46}$$

where we define T_c as the critical temperature.

The specific heat near the critical temperature for bosons is of great interest. For $0 < T < T_c$, we can practically use $z = 1$. The internal energy is then

$$U = \frac{3}{2}kT\frac{V}{\lambda^3}g_{5/2}(1) = \frac{3}{2}kT\frac{V}{\lambda^3}\zeta(5/2), \quad T < T_c. \tag{17.47}$$

Note that we cannot use equation (17.34) because N_0 is not zero. Based on the definition of equation (17.46),

$$\lambda = \left[\frac{\zeta(3/2)V}{N}\right]^{1/3}\left(\frac{T_c}{T}\right)^{1/2}, \tag{17.48}$$

we have

$$U = \frac{3}{2}NkT\left(\frac{T}{T_c}\right)^{3/2}\frac{\zeta(5/2)}{\zeta(3/2)}, \tag{17.49}$$

so the specific heat is

$$C_V = \left(\frac{\partial U}{\partial T}\right)_{N,V} = \frac{15}{4}Nk\left(\frac{T}{T_c}\right)^{3/2}\frac{\zeta(5/2)}{\zeta(3/2)} = 1.926Nk\left(\frac{T}{T_c}\right)^{3/2}, \quad T < T_c. \tag{17.50}$$

The specific heat at T_c is $1.926Nk$, which is significantly higher than the classical value $1.5Nk$.

Worksheet 17.5 The Riemann zeta function is defined as `Zeta`. After the definition of λ using equation (17.48), the calculations are straightforward.

```
> lambda := ((Tc/T)^(3/2)*(1/(N/(V*Zeta(3/2)))))^(1/3);
```

$$\lambda := \left(\frac{\left(\frac{Tc}{T} \right)^{(3/2)} V \zeta\left(\frac{3}{2} \right)}{N} \right)^{(1/3)}$$

```
> Eq1 := U = 3/2*k*T*V/lambda^3*Zeta(5/2);
```

$$Eq1 := U = \frac{3}{2} \frac{k T N \zeta\left(\frac{5}{2} \right)}{\left(\frac{Tc}{T} \right)^{(3/2)} \zeta\left(\frac{3}{2} \right)}$$

```
> Eq2 := C[V] = diff(rhs(Eq1), T):
> Eq3 := simplify(Eq2) assuming T>0;
```

$$Eq3 := C_V = \frac{15}{4} \frac{k T^{(3/2)} N \zeta\left(\frac{5}{2} \right)}{Tc^{(3/2)} \zeta\left(\frac{3}{2} \right)}$$

```
> Eq4 := evalf(Eq3);
```

$$Eq4 := C_V = \frac{1.925671675\, k T^{(3/2)} N}{Tc^{(3/2)}}$$

For $T > T_c$, setting $z = 1$ is no longer appropriate. From the graph of $g_{3/2}(z)$ versus z, we see that when z is near unity, it varies only weakly with $n\lambda^3$: z is thus not a convenient parameter. Instead we recall μ and devise an alternative parameter

$$\alpha = -\frac{\mu}{kT}. \tag{17.51}$$

According to this definition, α is a small positive number near the critical temperature, which is suitable for expansion.

The result for an expansion of $g_\sigma(\alpha)$, for which the derivation involves complex analysis, is

$$g_\sigma(\alpha) = \Gamma(1-\sigma)\alpha^{\sigma-1} + \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \zeta(\sigma - l)\alpha^l; \tag{17.52}$$

see Appendix B.4 for this derivation. For small α,

$$g_{3/2}(\alpha) \cong \Gamma(-1/2)\alpha^{1/2} + \zeta(3/2), \tag{17.53}$$

$$g_{5/2}(\alpha) \cong \Gamma(-3/2)\alpha^{3/2} + \zeta(5/2) - \zeta(3/2)\alpha. \tag{17.54}$$

Because

$$\frac{N}{V}\lambda^3 = g_{3/2}(\alpha) = \Gamma(-1/2)\alpha^{1/2} + \zeta(3/2), \tag{17.55}$$

we obtain α as a function of T:

$$\sqrt{\alpha} = \frac{\frac{N}{V}\lambda^3 - \zeta(3/2)}{\Gamma(-1/2)} = \frac{\zeta(3/2)}{2\sqrt{\pi}}\left[1 - \left(\frac{T_c}{T}\right)^{3/2}\right]. \tag{17.56}$$

Recall that

$$U = \frac{3}{2}NkT\frac{g_{5/2}(\alpha)}{g_{3/2}(\alpha)}; \tag{17.57}$$

we expand the function dependent on α that appears in U at small α,

$$\frac{g_{5/2}(\alpha)}{g_{3/2}(\alpha)} \cong \frac{\zeta(5/2)}{\zeta(3/2)} + \frac{2\sqrt{\pi}\zeta(5/2)}{\zeta(3/2)^2}\sqrt{\alpha} + \frac{-\zeta(3/2) + 4\frac{\zeta(5/2)\pi}{\zeta(3/2)^2}}{\zeta(3/2)}\alpha,$$

and eliminate α to obtain the internal energy,

$$\begin{aligned}\frac{U}{Nk} &= \frac{3T}{2}\frac{\zeta(5/2)}{\zeta(3/2)} + \frac{3T}{2}\frac{\zeta(5/2)}{\zeta(3/2)}\left[1 - \left(\frac{T_c}{T}\right)^{3/2}\right] \\ &\quad + \frac{3T}{2}\frac{1}{4\pi}\left[-\zeta(3/2)^2 + 4\frac{\zeta(5/2)\pi}{\zeta(3/2)}\right]\left[1 - \left(\frac{T_c}{T}\right)^{3/2}\right]^2, \quad T \gtrsim T_c. \end{aligned} \tag{17.58}$$

Differentiating U with respect to T, we find the specific heat to be

$$\begin{aligned}\frac{C_V}{Nk} &= \left[\frac{9}{2}\frac{\zeta(5/2)}{\zeta(3/2)} - \frac{3}{8}\frac{\zeta(3/2)^2}{\pi}\right] \\ &\quad + \left[\frac{9}{4}\frac{\zeta(5/2)}{\zeta(3/2)} - \frac{3}{8}\frac{\zeta(3/2)^2}{\pi}\right]\left(\frac{T_c}{T}\right)^{3/2} + \left[\frac{3}{4}\frac{\zeta(3/2)^2}{\pi} - \frac{3\zeta(5/2)}{\zeta(3/2)}\right]\left(\frac{T_c}{T}\right)^3 \\ &= 1.496 + 0.341\left(\frac{T_c}{T}\right)^{3/2} + 0.089\left(\frac{T_c}{T}\right)^3, \quad T \gtrsim T_c. \end{aligned} \tag{17.59}$$

This formula is valid for small α, or for T near T_c; at T_c,

$$\lim_{T\to T_c^+} C_V = \frac{15}{4}\frac{\zeta(5/2)}{\zeta(3/2)}Nk = 1.926Nk,$$

which is exactly the same value as that from equation (17.50). Even for higher temperature, C_V asymptotically approaches $1.496Nk$, which differs little from the supposed value $1.5Nk$ of the classical limit.

Worksheet 17.6 We use a symbol `u` to denote $\sqrt{\alpha}$ so that Maple does not need to assume the sign of α (we know that α is positive). The symbol `Epr2` signifies the ratio of $g_{5/2}(\alpha)$ to $g_{3/2}(\alpha)$, which we use their approximations in equations (17.54) and (17.53); we expand this ratio as a series of $\sqrt{\alpha}$ (symbol `u`), and retain three terms. The differentiation is similar to that in preceding worksheets.

```
> lambda := ((Tc/T)^(3/2)*(1/(N/(V*Zeta(3/2)))))^(1/3);
```

$$\lambda := \left(\frac{\left(\frac{Tc}{T} \right)^{(3/2)} V \zeta\left(\frac{3}{2} \right)}{N} \right)^{(1/3)}$$

```
> Eq1 := u = ((N/V*lambda^3 - Zeta(3/2))/(GAMMA(-1/2)));
```

$$Eq1 := u = -\frac{1}{2} \frac{\left(\frac{Tc}{T} \right)^{(3/2)} \zeta\left(\frac{3}{2} \right) - \zeta\left(\frac{3}{2} \right)}{\sqrt{\pi}}$$

```
> Epr2 := (GAMMA(-3/2)*u^3 + Zeta(5/2)
> - Zeta(3/2)*u^2)/(GAMMA(-1/2)*u + Zeta(3/2));
```

$$Epr2 := \frac{\frac{4\sqrt{\pi}\, u^3}{3} + \zeta\left(\frac{5}{2} \right) - \zeta\left(\frac{3}{2} \right) u^2}{-2\sqrt{\pi}\, u + \zeta\left(\frac{3}{2} \right)}$$

```
> Epr3 := convert(series(Epr2, u, 3), polynom);
```

$$Epr3 := \frac{\zeta\left(\frac{5}{2} \right)}{\zeta\left(\frac{3}{2} \right)} + \frac{2\zeta\left(\frac{5}{2} \right)\sqrt{\pi}\, u}{\zeta\left(\frac{3}{2} \right)^2} + \frac{\left(-\zeta\left(\frac{3}{2} \right) + \frac{4\zeta\left(\frac{5}{2} \right)\pi}{\zeta\left(\frac{3}{2} \right)^2} \right) u^2}{\zeta\left(\frac{3}{2} \right)}$$

```
> Epr4 := subs(Eq1, Epr3):
```

```
> Eq5 := U = 3/2*N*k*T*Epr4;
```

$$Eq5 := U = \frac{3}{2} N k T \left(\frac{\zeta\left(\frac{5}{2}\right)}{\zeta\left(\frac{3}{2}\right)} - \frac{\zeta\left(\frac{5}{2}\right) \left(\left(\frac{Tc}{T}\right)^{(3/2)} \zeta\left(\frac{3}{2}\right) - \zeta\left(\frac{3}{2}\right) \right)}{\zeta\left(\frac{3}{2}\right)^2} + \frac{1}{4} \frac{\left(-\zeta\left(\frac{3}{2}\right) + \frac{4\,\zeta\left(\frac{5}{2}\right) \pi}{\zeta\left(\frac{3}{2}\right)^2} \right) \left(\left(\frac{Tc}{T}\right)^{(3/2)} \zeta\left(\frac{3}{2}\right) - \zeta\left(\frac{3}{2}\right) \right)^2}{\zeta\left(\frac{3}{2}\right) \pi} \right)$$

```
> Eq6 := C[V] = diff(rhs(Eq5), T):
> Eq7 := simplify(Eq6) assuming T>0:
> Eq8 := expand(Eq7);
```

$$Eq8 := C_V = \frac{9}{2} \frac{N k \zeta\left(\frac{5}{2}\right)}{\zeta\left(\frac{3}{2}\right)} + \frac{9}{4} \frac{N k\, Tc^{(3/2)} \zeta\left(\frac{5}{2}\right)}{\zeta\left(\frac{3}{2}\right) T^{(3/2)}} + \frac{3}{4} \frac{N k \zeta\left(\frac{3}{2}\right)^2 Tc^3}{T^3 \pi} - \frac{3}{8} \frac{N k \zeta\left(\frac{3}{2}\right)^2 Tc^{(3/2)}}{T^{(3/2)} \pi} - \frac{3}{8} \frac{N k \zeta\left(\frac{3}{2}\right)^2}{\pi} - \frac{3\, N k \zeta\left(\frac{5}{2}\right) Tc^3}{\zeta\left(\frac{3}{2}\right) T^3}$$

```
> Eq9 := evalf(Eq8);
```

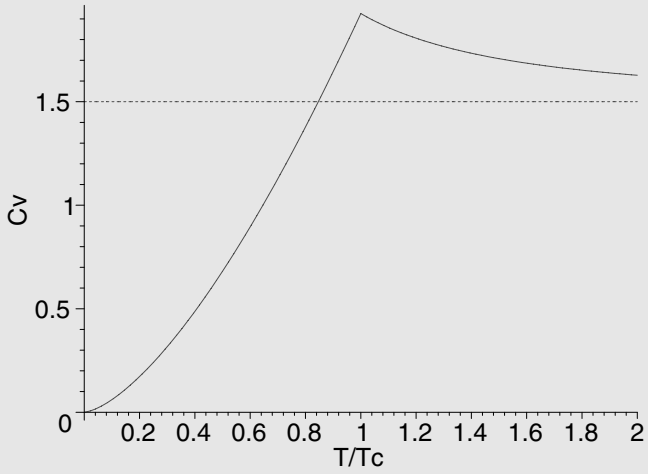
$$Eq9 := C_V = 1.496190736\, N k + \frac{0.3407877308\, N k\, Tc^{(3/2)}}{T^{(3/2)}} + \frac{0.088693208\, N k\, Tc^3}{T^3}$$

We plot the specific heat near the critical temperature.

Worksheet 17.7 We enter C_V for $T < T_c$ and $T > T_c$ and produce a plot; the classical $C_V = 1.5Nk$ is indicated.

```
> Cv1 := 1.926*T^(3/2):
> Cv2 := 1.496 + 0.341*(1/T)^(3/2) + 0.089*(1/T)^3:
> with(plots):
Warning, the name changecoords has been redefined
```

```
> p1 := plot(Cv1, T=0..1):
> p2 := plot(Cv2, T=1..2):
> p3 := plot(1.5, T=0..2, linestyle=4):
> display([p1, p2, p3]);
```



This plot shows that the shape of the curve for the specific heat resembles the Greek letter λ; for this reason the critical temperature is commonly called the lambda point. Notice that the value of the specific heat is continuous at T_c, but its derivative is discontinuous. The calculation of the discontinuity is left as an exercise at the end of the chapter.

17.4 Ideal Fermi Gas

The distribution for Fermi–Dirac statistics is

$$\overline{n}_\varepsilon = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}. \tag{17.60}$$

The maximum value of $\overline{n}_\varepsilon$ is 1, but there is no restriction on μ: it can be negative or positive.

Much mathematics required for Fermi–Dirac statistics is similar to that for Bose–Einstein statistics, with one distribution replacing the other. The number of particles is

$$N = \frac{gV(4\sqrt{2}\pi m^{3/2})}{h^3}\int_0^\infty \frac{\varepsilon^{1/2}}{e^{\beta(\epsilon-\mu)}+1}d\varepsilon, \tag{17.61}$$

and the internal energy is

$$U = \frac{gV(4\sqrt{2}\pi m^{3/2})}{h^3} \int_0^\infty \frac{\varepsilon^{3/2}}{e^{\beta(\epsilon-\mu)}+1} d\varepsilon. \tag{17.62}$$

We include the number g of possible spin orientations in our equations.

Adopting the same definitions of λ, x and z as for an ideal Bose gas, and defining the Fermi–Dirac integral function,

$$f_\sigma(z) = \frac{1}{\Gamma(\sigma)} \int_0^\infty \frac{x^{\sigma-1}}{z^{-1}e^x + 1}\, dx, \tag{17.63}$$

we write

$$N = \frac{gV}{\lambda^3} f_{3/2}(z), \tag{17.64}$$

$$U = \frac{3}{2} kT \frac{f_{5/2}(z)}{f_{3/2}(z)}, \tag{17.65}$$

$$P = \frac{NkT}{V} \frac{f_{5/2}(z)}{f_{3/2}(z)}. \tag{17.66}$$

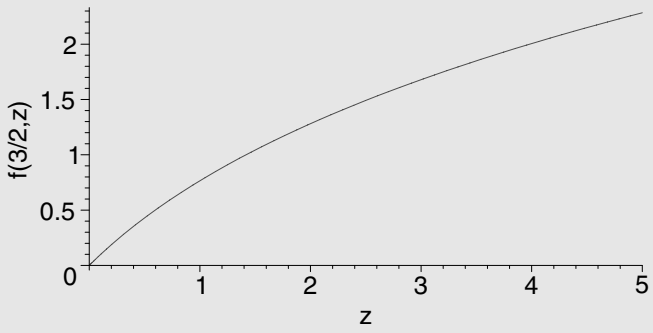
These integrals likewise yield no analytic expression. All quantities are expressed in terms of z; again we require z as a function of N, V and T. In principle, we can adopt the graphical approach as presented for Bose–Einstein statistics. Because there is no restriction on μ, the range of z can include any positive value $0 < z < \infty$.

Worksheet 17.8 This worksheet is similar to that for Bose–Einstein statistics.

```
> f := (sigma, z) -> int(x^(sigma-1)/(exp(x)/z + 1),
> x=0..infinity)/GAMMA(sigma);
```

$$f := (\sigma,\, z) \to \frac{1}{\Gamma(\sigma)} \int_0^\infty \frac{x^{(\sigma-1)}}{\frac{e^x}{z} + 1}\, dx$$

```
> plot(f(3/2,z), z=0..5, scaling=constrained);
```



Our objective to find $f_{3/2}^{-1}$, so that

$$z = f_{3/2}^{-1}(n\lambda^3/g),$$

is accomplished numerically from the graph. The conduction electrons in a metal at room temperature is an example of an ideal Fermi gas; we leave it to an exercise to find the chemical potential of metallic silver by the graphical method.

For small z, $f_{3/2}(z)$ exhibits a linear relation, like $g_{3/2}(z)$; thus an ideal Fermi gas also reduces to the classical limit at low density. For the condition $n\lambda^3 < 1$, we can employ the virial expansion similar to that for an ideal Bose gas, which we will discuss in Section 17.4.1.

The behavior of an ideal Fermi gas at low temperature differs greatly from that of an ideal Bose gas. In conformity with Pauli's exclusion principle, occupation of a single quantum state by more than one particle does not occur. The phenomena exhibited by an ideal Fermi gas is the subject of Section 17.4.2.

17.4.1 Low Density and Virial Expansion

The condition for low density is that

$$\frac{n\lambda^3}{g} < 1.$$

The treatment of an ideal Fermi gas at low density is identical to that of an ideal Bose gas at low density, except that we replace the function $g_\sigma(z)$ with $f_\sigma(z)$. Virial coefficients for a

Fermi gas have the same values as for a Bose gas except for the alternating sign of consecutive terms.

We list the results here, but leave the derivation to an exercise. The equation of state is expressed as

$$\frac{P}{nkT} = 1 + a_1\left(\frac{n\lambda^3}{g}\right) + a_2\left(\frac{n\lambda^3}{g}\right)^2 + a_3\left(\frac{n\lambda^3}{g}\right)^3 + \ldots, \tag{17.67}$$

where

$$\begin{aligned} a_1 &= 0.17678, \\ a_2 &= -0.0033, \\ a_3 &= 0.00011. \end{aligned} \tag{17.68}$$

The specific heat is

$$\frac{C_V}{N} = \frac{3}{2}k\left[1 - 0.084\left(\frac{n\lambda^3}{g}\right) + 0.0066\left(\frac{n\lambda^3}{g}\right)^2 - 0.0004\left(\frac{n\lambda^3}{g}\right)^3 + \ldots\right]. \tag{17.69}$$

17.4.2 Specific Heat of a Metal at Low Temperature

The context of low temperature in this subsection is that

$$\mu \gg kT.$$

In this regime, the fugacity z is no longer a convenient parameter: we return to the original expression of μ. In the limit when $T \to 0$, the distribution becomes a step function,

$$\overline{n}_\varepsilon = \begin{cases} 1, & \varepsilon < \mu_0, \\ 0, & \varepsilon > \mu_0. \end{cases}$$

At zero temperature the chemical potential μ_0 is the Fermi energy, denoted by ε_F.

The Fermi energy is readily calculable. Because at 0 K all states are filled below ε_F, but are completely empty above that energy, the number of particles is

$$N = \frac{gV}{h^3}\int_0^{\varepsilon_F} 4\sqrt{2}\pi m^{3/2}\varepsilon^{1/2}d\varepsilon, \tag{17.70}$$

and the ground state energy is

$$U_0 = \frac{gV}{h^3}\int_0^{\varepsilon_F} 4\sqrt{2}\pi m^{3/2}\varepsilon^{3/2}d\varepsilon. \tag{17.71}$$

We leave it to an exercise to verify that the Fermi energy is

$$\varepsilon_F = \left(\frac{3N}{4\pi g V}\right)^{2/3} \frac{h^2}{2m}. \tag{17.72}$$

The internal energy, expressed in terms of the Fermi energy, is

$$U_0 = \frac{3}{5} N \varepsilon_F; \tag{17.73}$$

the pressure at 0 K is thus

$$P_0 = \frac{2}{3}\frac{U_0}{V} = \frac{2}{5}\frac{N}{V}\varepsilon_F. \tag{17.74}$$

A Fermi system is active even at absolute zero of temperature.

We plot the distribution for Fermi–Dirac statistics at low temperature when μ is sufficiently large relative to kT.

Worksheet 17.9 To produce such a plot, we choose an arbitrarily large number for μ, for instance $50\,000\,k$.

```
> nfd := 1/(exp(beta*(En - mu)) + 1);
```

$$nfd := \frac{1}{e^{(\beta\,(En-\mu))}+1}$$

```
> mu := 50000;
```

$$\mu := 50000$$

```
> nfd1000 := eval(nfd, beta=1/1000);
```

$$nfd1000 := \frac{1}{e^{(\frac{En}{1000}-50)}+1}$$

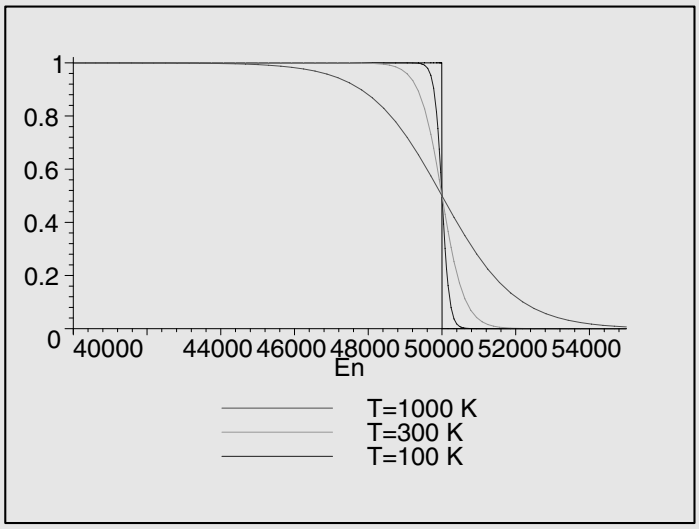
```
> nfd300 := eval(nfd, beta=1/300);
```

$$nfd300 := \frac{1}{e^{(\frac{En}{300}-500/3)}+1}$$

```
> nfd100 := eval(nfd, beta=1/100);
```

$$nfd100 := \frac{1}{e^{(\frac{En}{100}-500)}+1}$$

```
> plot([nfd1000, nfd300, nfd100, 1 - Heaviside(En-mu)],
> En=mu-10000..mu+5000, legend=["T=1000 K", "T=300 K", "T=100 K",
> "T=0 K"]);
```



According to this plot, n_ε decreases abruptly from 1 to 0 within a narrow range about $\varepsilon = \mu$, but is nearly constant elsewhere.

The number of particles is

$$N = \frac{gV(4\sqrt{2}\pi m^{3/2})}{h^3} \int_0^\infty \frac{\varepsilon^{1/2}}{e^{\beta(\epsilon-\mu)}+1} d\varepsilon, \tag{17.75}$$

and the internal energy is

$$U = \frac{gV(4\sqrt{2}\pi m^{3/2})}{h^3} \int_0^\infty \frac{\varepsilon^{3/2}}{e^{\beta(\epsilon-\mu)}+1} d\varepsilon. \tag{17.76}$$

Both these quantities appear in an integral of this form:

$$I_s = \int_0^\infty \frac{\varepsilon^s}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon. \tag{17.77}$$

We expand I_s as

$$I_s = \int_0^\mu \varepsilon^s d\varepsilon - \int_0^\mu \left[1 - \frac{1}{e^{\beta(\varepsilon-\mu)}+1}\right] \varepsilon^s d\varepsilon + \int_\mu^\infty \frac{\varepsilon^s}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon. \tag{17.78}$$

We interpret these integrals as follows: the first signifies the step function, which gives the major contribution; the second and third constitute deviations from that step function.

Introducing a parameter η,

$$\eta = \beta(\varepsilon - \mu), \tag{17.79}$$

we find that the third integral above becomes

$$\int_{\mu}^{\infty} \frac{\varepsilon^s}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon = kT \int_0^{\infty} \frac{(\mu+kT\eta)^s}{e^{\eta}+1} d\eta.$$

For the second integral, we first express a deviation from the step function as

$$1 - \frac{1}{e^{\beta(\varepsilon-\mu)}+1} = \frac{e^{\beta(\varepsilon-\mu)}}{e^{\beta(\varepsilon-\mu)}+1} = \frac{1}{e^{\beta(\mu-\varepsilon)}+1}.$$

Introducing another parameter η',

$$\eta' = \beta(\mu - \varepsilon),$$

we find that the second integral becomes

$$\int_0^{\mu} \left[1 - \frac{1}{e^{\beta(\varepsilon-\mu)}+1}\right] \varepsilon^s d\varepsilon = -kT \int_{\mu/kT}^{0} \frac{(\mu - kT\eta')^s}{e^{\eta'}+1} d\eta' \cong kT \int_0^{\infty} \frac{(\mu - kT\eta')^s}{e^{\eta'}+1} d\eta'.$$

As this approximation is based on our condition of interest, $\mu \gg kT$, we replace μ/kT by ∞. The expanded integral becomes

$$I_s = \int_0^{\mu} \varepsilon^s d\varepsilon + kT \int_0^{\infty} \frac{(\mu+kT\eta)^s - (\mu-kT\eta)^s}{e^{\eta}+1} d\eta. \tag{17.80}$$

The deviation from a step function is appreciable only when ε is near μ, such that for only small η is there a significant contribution; we expand the integral as a series. Defining

$$\varphi(\eta) = (\mu + kT\eta)^s - (\mu - kT\eta)^s,$$

we write

$$\varphi(\eta) = 1 + \left(\frac{\partial\varphi}{\partial\eta}\right)_{\eta=0} \eta + \frac{1}{2!}\left(\frac{\partial^2\varphi}{\partial\eta^2}\right)_{\eta=0} \eta^2 + \frac{1}{3!}\left(\frac{\partial^3\varphi}{\partial\eta^3}\right)_{\eta=0} \eta^3 + \ldots.$$

Coefficients

$$\left(\frac{\partial^l\varphi}{\partial\eta^l}\right)_{\eta=0}$$

are a function of μ; integral I therefore takes the form

$$\int_0^{\infty} \frac{\eta^l}{e^{\eta}+1} d\eta,$$

which is readily evaluated with Maple. We have

$$\begin{aligned} N &= \frac{gV(4\sqrt{2}\pi m^{3/2})}{h^3} I_{1/2} \\ &= \frac{4\pi gV}{3}\left(\frac{2m}{h^2}\right)^{3/2} \mu^{3/2}\left[1 + \frac{1}{8}\left(\frac{\pi kT}{\mu}\right)^2 + \frac{7}{640}\left(\frac{\pi kT}{\mu}\right)^4 \ldots\right], \end{aligned} \tag{17.81}$$

$$\begin{aligned} U &= \frac{gV(4\sqrt{2}\pi m^{3/2})}{h^3} I_{3/2} \\ &= \frac{4\pi gV}{3}\left(\frac{2m}{h^2}\right)^{3/2}\frac{3}{5}\mu^{5/2}\left[1+\frac{5}{8}\left(\frac{\pi kT}{\mu}\right)^2-\frac{7}{384}\left(\frac{\pi kT}{\mu}\right)^4+\ldots\right]. \end{aligned} \tag{17.82}$$

To express μ in terms of N/V and T, we again take progressive steps until we attain the desired precision. At zeroth order,

$$\frac{4\pi g}{3}\left(\frac{2m}{h^2}\right)^{3/2}\mu^{3/2} \cong \frac{N}{V}, \quad \mu \cong \left(\frac{3N}{4\pi gV}\right)^{2/3}\frac{h^2}{2m} = \varepsilon_F.$$

This result is identical to equation (17.72), which applies to a Fermi system at absolute zero of temperature. In the next approximation, we have

$$\frac{4\pi g}{3}\left(\frac{2m}{h^2}\right)^{3/2}\mu^{3/2} \cong \frac{N}{V}\left[1+\frac{1}{8}\left(\frac{\pi kT}{\varepsilon_F}\right)^2\right]^{-1}, \quad \mu \cong \varepsilon_F\left[1+\frac{1}{8}\left(\frac{\pi kT}{\varepsilon_F}\right)^2\right]^{-2/3}.$$

We then expand μ as a series of ε_F:

$$\mu = \varepsilon_F\left[1-\frac{\pi^2}{12}\left(\frac{kT}{\varepsilon_F}\right)^2\right]. \tag{17.83}$$

Applying this expression to eliminate μ from U/N, we proceed to expand it at $\varepsilon_F = \infty$; the result is

$$\frac{U}{N} = \frac{I_{3/2}}{I_{1/2}} = \frac{3}{5}\varepsilon_F\left[1+\frac{5\pi^2}{12}\left(\frac{kT}{\varepsilon_F}\right)^2\right]. \tag{17.84}$$

The pressure remains two-thirds of the energy density,

$$P = \frac{2}{3}\frac{U}{V} = \frac{2}{5}\frac{N}{V}\varepsilon_F\left[1+\frac{5\pi^2}{12}\left(\frac{kT}{\varepsilon_F}\right)^2\right], \tag{17.85}$$

and the specific heat is

$$\frac{C_V}{N} = \frac{\pi^2}{2}\frac{kT}{\varepsilon_F}. \tag{17.86}$$

Worksheet 17.10 The integrands of equation (17.80) are defined as `phi1` and `phi2`, respectively. After expanding the integrands in a Taylor series at $\eta = 0$, we evaluate the integral of equation (17.80): `Eye[1/2]` is for $I_{1/2}$ and `Eye[3/2]` is for $I_{3/2}$. With regard to finding the chemical potential μ, `Eq13` is the zeroth order, and `Eq15` the first order; μ is solved in `Eq16`. To expand μ as a series of ε_F, in `Eq17` we use the `series` command and set ε_F at infinity. In `Eq33`, again we expand U/N at $\varepsilon_F = \infty$.

```
> assume(k>0, T>0, mu>0);
> phi1 := s -> epsilon^s;
```

$$\phi 1 := s \to \varepsilon^s$$

```
> phi2 := (s,eta) -> (mu + k*T*eta)^s - (mu - k*T*eta)^s;
```

$$\phi 2 := (s,\, \eta) \to (\mu + k\,T\,\eta)^s - (\mu - k\,T\,\eta)^s$$

```
> Epr1 := convert(taylor(phi2(1/2, eta), eta=0, 4), polynom);
```

$$Epr1 := \frac{k\,T\,\eta}{\sqrt{\mu}} + \frac{k^3\,T^3\,\eta^3}{8\,\mu^{(5/2)}}$$

```
> Epr2 := convert(taylor(phi2(3/2, eta), eta=0, 4), polynom);
```

$$Epr2 := 3\,\sqrt{\mu}\,k\,T\,\eta - \frac{k^3\,T^3\,\eta^3}{8\,\mu^{(3/2)}}$$

```
> Eye[1/2] := int(phi1(1/2), epsilon=0..mu) +
> k*T*(int(expand(Epr1/(exp(eta) + 1)), eta=0..infinity));
```

$$Eye_{1/2} := \frac{2\,\mu^{(3/2)}}{3} + k\,T\,\left(\frac{k\,T\,\pi^2}{12\,\sqrt{\mu}} + \frac{7\,k^3\,T^3\,\pi^4}{960\,\mu^{(5/2)}}\right)$$

```
> Eye[3/2] := int(phi1(3/2), epsilon=0..mu) +
> k*T*(int(expand(Epr2/(exp(eta) + 1)), eta=0..infinity));
```

$$Eye_{3/2} := \frac{2\,\mu^{(5/2)}}{5} + k\,T\,\left(\frac{\sqrt{\mu}\,k\,T\,\pi^2}{4} - \frac{7\,k^3\,T^3\,\pi^4}{960\,\mu^{(3/2)}}\right)$$

```
> Eq5 := N = g*V*4*sqrt(2)*m^(3/2)*Pi/h^3*Eye[1/2];
```

$$Eq5 := N = \frac{4\,g\,V\,\sqrt{2}\,m^{(3/2)}\,\pi\,\left(\frac{2\,\mu^{(3/2)}}{3} + k\,T\,\left(\frac{k\,T\,\pi^2}{12\,\sqrt{\mu}} + \frac{7\,k^3\,T^3\,\pi^4}{960\,\mu^{(5/2)}}\right)\right)}{h^3}$$

```
> Epr11 := g*V*4*sqrt(2)*m^(3/2)*Pi/h^3*(int(phi1(1/2),
> epsilon=0..mu));
```

$$Epr11 := \frac{8\,g\,V\,\sqrt{2}\,m^{(3/2)}\,\pi\,\mu^{(3/2)}}{3\,h^3}$$

```
> Epr12 := g*V*4*sqrt(2)*m^(3/2)*Pi/h^3
> *(k*T*(int(op(1,Epr1)/(exp(eta) + 1), eta=0..infinity)));
```

$$Epr12 := \frac{g\,V\,\sqrt{2}\,m^{(3/2)}\,\pi^3\,k^2\,T^2}{3\,h^3\,\sqrt{\mu}}$$

```
> Eq13 := N = subs(mu=epsilon[F], Epr11);
```

$$Eq13 := N = \frac{8}{3}\,\frac{g\,V\,\sqrt{2}\,m^{(3/2)}\,\pi\,{\varepsilon_F}^{(3/2)}}{h^3}$$

```
> Epr14 := simplify(Epr12/Epr11);
```

$$Epr14 := \frac{\pi^2\, k^2\, T^2}{8\,\mu^2}$$

```
> Eq15 := Epr11 = subs({Eq13, mu=epsilon[F]}, N/(1 + Epr14));
```

$$Eq15 := \frac{8\,g\,V\,\sqrt{2}\,m^{(3/2)}\,\pi\,\mu^{(3/2)}}{3\,h^3} = \frac{8}{3}\,\frac{g\,V\,\sqrt{2}\,m^{(3/2)}\,\pi\,{\varepsilon_F}^{(3/2)}}{h^3\left(1+\frac{1}{8}\,\frac{\pi^2\,k^2\,T^2}{{\varepsilon_F}^2}\right)}$$

```
> Eq16 := isolate(Eq15, mu);
```

$$Eq16 := \mu = \left(\frac{{\varepsilon_F}^{(3/2)}}{1+\frac{1}{8}\,\frac{\pi^2\,k^2\,T^2}{{\varepsilon_F}^2}}\right)^{(2/3)}$$

```
> Eq17 := mu = convert(series(rhs(Eq16), epsilon[F]=infinity, 3),
> polynom);
```

$$Eq17 := \mu = \varepsilon_F - \frac{1}{12}\,\frac{\pi^2\,k^2\,T^2}{\varepsilon_F}$$

```
> Eq31 := U/N = Eye[3/2]/Eye[1/2];
```

$$Eq31 := \frac{U}{N} = \frac{\frac{2\,\mu^{(5/2)}}{5} + k\,T\left(\frac{\sqrt{\mu}\,k\,T\,\pi^2}{4} - \frac{7\,k^3\,T^3\,\pi^4}{960\,\mu^{(3/2)}}\right)}{\frac{2\,\mu^{(3/2)}}{3} + k\,T\left(\frac{k\,T\,\pi^2}{12\,\sqrt{\mu}} + \frac{7\,k^3\,T^3\,\pi^4}{960\,\mu^{(5/2)}}\right)}$$

```
> Eq32 := subs(Eq16, Eq31);
```

$$Eq32 := \frac{U}{N} = \frac{\frac{2}{5}\left(\frac{{\varepsilon_F}^{(3/2)}}{\%1}\right)^{(5/3)} + k\,T\left(\frac{1}{4}\left(\frac{{\varepsilon_F}^{(3/2)}}{\%1}\right)^{(1/3)} k\,T\,\pi^2 - \frac{7}{960}\,\frac{\%1\,k^3\,T^3\,\pi^4}{{\varepsilon_F}^{(3/2)}}\right)}{\frac{2}{3}\,\frac{{\varepsilon_F}^{(3/2)}}{\%1} + k\,T\left(\frac{1}{12}\,\frac{k\,T\,\pi^2}{\left(\frac{{\varepsilon_F}^{(3/2)}}{\%1}\right)^{(1/3)}} + \frac{7}{960}\,\frac{k^3\,T^3\,\pi^4}{\left(\frac{{\varepsilon_F}^{(3/2)}}{\%1}\right)^{(5/3)}}\right)}$$

$$\%1 := 1 + \frac{1}{8}\,\frac{\pi^2\,k^2\,T^2}{{\varepsilon_F}^2}$$

```
> Eq33 := lhs(Eq32) = convert(series(rhs(Eq32),
> epsilon[F]=infinity, 3), polynom);
```

$$Eq33 := \frac{U}{N} = \frac{3}{5}\,\varepsilon_F + \frac{1}{4}\,\frac{\pi^2\,k^2\,T^2}{\varepsilon_F}$$

```
> Eq34 := P = expand(2/3*N/V*rhs(Eq33));
```

$$Eq34 := P = \frac{2}{5}\frac{N\,\varepsilon_F}{V} + \frac{1}{6}\frac{N\,\pi^2\,k^2\,T^2}{V\,\varepsilon_F}$$

```
> Eq35 := C[V]/N = diff(rhs(Eq33), T);
```

$$Eq35 := \frac{C_V}{N} = \frac{1}{2}\frac{\pi^2\,k^2\,T}{\varepsilon_F}$$

As mentioned, conduction electrons in a metal can be modeled as an ideal Fermi gas. At low temperature, the specific heat C_V of a metal at constant volume is linearly proportional to T.

17.5 Relativistic Gases

Quantum statistics is applicable to extremely relativistic particles at high density. Such a condition would have occurred within seconds after the *big bang*. At this limit, the integrals can be evaluated exactly.

According to special relativity as explained in Chapter 12, the relation between energy and momentum is

$$\varepsilon^2 = (mc^2)^2 + (pc)^2. \tag{17.87}$$

Ignoring the rest mass m of the particle, we express the energy of an extremely relativistic particle as

$$\varepsilon = pc. \tag{17.88}$$

The element of momentum space is readily derived as

$$d^3p = 4\pi p^2 dp = \frac{4\pi\varepsilon^2}{c^3}d\varepsilon.$$

Our concern here is with a temperature that is extremely high; under such a condition we ignore the chemical potential,

$$\frac{\varepsilon-\mu}{kT} \cong \frac{\varepsilon}{kT}.$$

Applying the formulation of quantum statistics, we directly perform an integration to obtain our desired quantities. For bosons,

$$N = \frac{gV}{h^3}\int_0^\infty \frac{1}{e^{\varepsilon/kT}-1}\frac{4\pi\varepsilon^2}{c^3}d\varepsilon = \frac{8gV\pi k^3T^3\zeta(3)}{h^3c^3}, \tag{17.89}$$

where $\zeta(3) = 1.202$ is again the Riemann zeta function.

The internal energy is

$$U = \frac{gV}{h^3}\int_0^\infty \frac{\varepsilon}{e^{\varepsilon/kT}-1}\frac{4\pi\varepsilon^2}{c^3}d\varepsilon = \frac{4gV\pi^5k^4T^4}{15h^3c^3}. \tag{17.90}$$

From equation (17.12), we calculate

$$\frac{p}{3}\frac{d\varepsilon}{dp} = \frac{1}{3}\varepsilon;$$

for a relativistic gas, the pressure is therefore one-third of the energy density:

$$P = \frac{1}{3}\frac{U}{V} = \frac{1}{3}\frac{4g\pi^5k^4T^4}{15h^3c^3}. \tag{17.91}$$

We perform the same calculations for fermions, using the corresponding distribution. The number of particles is

$$N = \frac{gV}{h^3}\int_0^\infty \frac{1}{e^{\varepsilon/kT}+1}\frac{4\pi\varepsilon^2}{c^3}d\varepsilon = \frac{3}{4}\frac{8gV\pi k^3T^3\zeta(3)}{h^3c^3}, \tag{17.92}$$

and the energy is

$$U = \frac{gV}{h^3}\int_0^\infty \frac{\varepsilon}{e^{\varepsilon/kT}+1}\frac{4\pi\varepsilon^2}{c^3}d\varepsilon = \frac{7}{8}\frac{4gV\pi^5k^4T^4}{15h^3c^3}; \tag{17.93}$$

the pressure is still one-third of the energy density

$$P = \frac{1}{3}\frac{U}{V} = \frac{1}{3}\frac{7}{8}\frac{4g\pi^5k^4T^4}{15h^3c^3}. \tag{17.94}$$

Worksheet 17.11 To evaluate all integrals above with Maple, we must specify the sign of k, T and c, using the `assume` command. The symbols `nbe`, `nfd` and `Epr1` signify the Bose–Einstein distribution, the Fermi–Dirac distribution and the element of momentum space, respectively. All the integrals are evaluated analytically, with results containing the Riemann zeta function.

```
> assume(k>0, T>0, c>0);
> nbe := 1/(exp(epsilon/(k*T)) - 1);
```

$$nbe := \frac{1}{e^{(\frac{\varepsilon}{kT})}-1}$$

```
> nfd := 1/(exp(epsilon/(k*T)) + 1);
```

$$nfd := \frac{1}{e^{(\frac{\varepsilon}{kT})}+1}$$

```
> p := epsilon/c;
```

$$p := \frac{\varepsilon}{c}$$

```
> Epr1 := 4*Pi*p^2*diff(p, epsilon);
```

$$Epr1 := \frac{4\,\pi\,\varepsilon^2}{c^3}$$

```
> Eq11 := En =g*V/h^3*int(nbe*epsilon*Epr1, epsilon=0..infinity);
```

$$Eq11 := En = \frac{4\,g\,V\,\pi^5\,k^4\,T^4}{15\,h^3\,c^3}$$

```
> Eq12 := N = g*V/h^3*int(nbe*Epr1, epsilon=0..infinity);
```

$$Eq12 := N = \frac{8\,g\,V\,\pi\,k^3\,T^3\,\zeta(3)}{h^3\,c^3}$$

```
> Eq13 := En = g*V/h^3*int(nfd*epsilon*Epr1, epsilon=0..infinity);
```

$$Eq13 := En = \frac{7\,g\,V\,\pi^5\,k^4\,T^4}{30\,h^3\,c^3}$$

```
> Eq14 := N = g*V/h^3*int(nfd*Epr1, epsilon=0..infinity);
```

$$Eq14 := N = \frac{6\,g\,V\,\pi\,k^3\,T^3\,\zeta(3)}{h^3\,c^3}$$

The chemical potential of a photon is zero; the Bose–Einstein distribution under such a condition ($\mu = 0$) is called the Planck distribution. A photon has spin 1 and no rest mass. The above calculations for bosons are applicable to photons at any temperature and density. Although a particle of spin 1 has three possible orientations of that intrinsic angular momentum, for a photon $g = 2$, because the photon is polarized perpendicular to its direction of propagation; this condition eliminates one degree of freedom. The energy density for a photon is then

$$\frac{U}{V} = \frac{8\pi^5 k^4 T^4}{15 h^3 c^3}, \tag{17.95}$$

or the net flow of radiation per unit area of an aperture is

$$R_T = \frac{c}{4}\frac{U}{V} = \frac{2\pi^5 k^4}{15 h^3 c^2} T^4 \equiv \sigma T^4, \tag{17.96}$$

which is the Stefan–Boltzmann law for radiation from a blackbody at temperature T. From equation (17.90), we obtain the energy spectrum,

$$\rho_T d\varepsilon = \frac{8\pi}{c^3 h^3} \frac{\varepsilon^3}{e^{\varepsilon/kT} - 1} d\varepsilon, \tag{17.97}$$

where

$$\varepsilon = h\nu. \tag{17.98}$$

Applying quantum statistics thus enables one to derive the spectral distribution of the blackbody radiation.

Equations (17.90) for bosons and (17.93) for fermions differ by a factor: a fermion contributes $7/8$ as much energy as a boson. Making use of the thermodynamic identity

$$U - TS + PV \equiv N\mu, \tag{17.99}$$

we find the entropy to be

$$S = \frac{U + PV}{T}, \tag{17.100}$$

for $\mu = 0$. Because both U and PV are proportional to T^4, entropy per unit volume is proportional to T^3:

$$\frac{S}{V} = \frac{2}{3} N_T \frac{8\pi^5 k^4}{15h^3c^3} T^3, \tag{17.101}$$

where N_T is defined as the effective number of species:

$$N_T = \begin{cases} f \times g \times 1, & \text{for a boson,} \\ f \times g \times \frac{7}{8}, & \text{for a fermion.} \end{cases} \tag{17.102}$$

This quantity gives the relative contribution of each type of particle to the total energy, pressure and entropy. We calculate the effective number of species N_T as a product of three factors: the first factor f is 2 or 1 depending whether the particle has or lacks an anti-particle; the second factor g specifies the number of possible spin orientations, and the third factor takes into account whether the particle is a boson or a fermion: the former is counted as 1, and the latter $7/8$.

As mentioned earlier, extremely relativistic conditions would have occurred moments after the big bang. Results in this section are pertinent to the cosmology of the early universe. For an interested reader, *The First Three Minutes*[2] is highly recommended. According to the standard model of cosmology, the universe in its present phase began with a singularity, commonly called the big bang; for details see Section 18.4.1. Within one second after the big bang, the universe was an extremely hot and dense plasma in a state of nearly perfect thermal equilibrium. Major constituents of that plasma in thermal equilibrium were photons, electrons, positrons, neutrinos and anti-neutrinos. The universe expanded and cooled, and about one second after the big bang neutrinos and anti-neutrinos left that thermal equilibrium with photons, electrons and positrons because their interactions are too weak to allow them to transfer energy to and from other particles. About 10 seconds after the big bang, as the universe was not hot enough for pair production of electrons and positrons, they rapidly disappeared. The expansion of the universe is an adiabatic process, for which the entropy remains constant. Annihilation of electrons and positrons decreased the effective number of species. According to equation (17.101), if N_T decreases, T must increase to maintain the same entropy.

Because neutrinos were already decoupled from the system, the effective number of species before annihilation was

$$N_{\text{before}} = 2 \times 2 \times \frac{7}{8} + 1 \times 2 \times 1 = \frac{11}{2}.$$

[2] S. Weinberg, *The First Three Minutes*, New York: Basic Books, 1993, Chapter V and Note 6.

The first term of this formula pertains to electrons and positrons, the second term to photons; see equation (17.102).

After annihilation, there remained only photons,

$$N_{\text{after}} = 2.$$

Annihilation clearly reheated the system, consisting then of only photons, by a factor

$$\frac{T_{\text{after}}}{T_{\text{before}}} = \left(\frac{11}{4}\right)^{1/3} = 1.401.$$

The residual heat of the early universe is detected as a cosmic microwave background at 2.73 K; this observation provides strong evidence in favor of the big-bang model. The residual heat is also expected to be manifest as the cosmic neutrino background. Because neutrinos did not benefit from reheating during electron–positron annihilation, their temperature is expected to be $1/1.401$ that of photons, or 1.95 K. As neutrinos are fermions, their energy spectrum is expected to appear as

$$\rho_T d\varepsilon = \frac{4\pi}{c^3 h^3} \frac{\varepsilon^3}{e^{\varepsilon/kT} + 1} d\varepsilon. \tag{17.103}$$

This formula differs from that for blackbody radiation, with Fermi–Dirac statistics replacing Bose–Einstein statistics. We leave it to the reader to plot such a spectrum. With present and foreseeable future technology, it will be a daunting task to detect the cosmic neutrino background at 1.95 K.

Exercises

1. At 4 K, the density of liquid ^{4}He is 0.129 g cm^{-3}, and its atomic mass is 4 u.

   (a) Verify that the particle density is 1.94×10^{28} m^{-3}.

   (b) Find the λ point for ^{4}He treated as an ideal Bose gas using equation (17.46).

   (c) Use equation (17.32′) to obtain z of liquid ^{4}He at 4 K with Maple's `fsolve` command.

2. Using equations (17.50) and (17.59), verify that the discontinuity of the specific heat at the λ point is

$$\left(\frac{\partial C_V}{\partial T}\right)_{T_c^-} - \left(\frac{\partial C_V}{\partial T}\right)_{T_c^+} = \frac{27Nk\zeta(3/2)^2}{16\pi T_c}. \tag{17.104}$$

3. The exact specific heat of an ideal Bose gas is given by an implicit formula:[3]

$$\frac{C_V}{Nk} = \frac{15}{4}\frac{g_{5/2}(z)}{g_{3/2}(z)} - \frac{9}{4}\frac{g_{3/2}(z)}{g_{1/2}(z)}. \tag{17.105}$$

   Recall that $n\lambda^3 = \zeta(3/2)$ at T_c, and $n\lambda^3 \propto T^{-3/2}$ with N and V fixed. Use equation (17.32′) to find z at $1.5\,T_c$, $2.0\,T_c$ and $3\,T_c$ with `fsolve`, so as to obtain C_V at these temperatures; compare the results with those from equation (17.59).
   Answer: the numerical method gives $1.71034\,Nk$ at $1.5\,T_c$, $1.63138\,Nk$ at $2.0\,T_c$ and $1.56923\,Nk$ at $3.0\,T_c$.

4. Treating conduction electrons in silver as an ideal Fermi gas, apply the graphical method (equation (17.64)) to find z and μ. The density of silver is 10.5 g cm^{-3}, and its atomic mass is 108 u; there is effectively one free electron per atom. Verify that the particle density is 5.85×10^{28} m^{-3}, and estimate z and μ at 300 K.
   Hint: because there is no restriction on z, application of the graphical method is awkward and the `fsolve` command is inefficient. Than range of z is between 10^{92} and 10^{93}, and μ from numerical solution is 5.51 eV. A much better way to find μ is to use equation (17.83).

5. Evaluate virial coefficients for an ideal Fermi gas.

6. Verify equations (17.72), (17.73) and (17.74) for chemical potential, internal energy and pressure at absolute zero.

7. Obtain one more term for the chemical potential and the internal energy of a degenerate Fermi gas in equation (17.83) and (17.84); show that in the second approximation,

$$\mu = \varepsilon_F \left[1 - \frac{\pi^2}{12}\left(\frac{kT}{\varepsilon_F}\right)^2 - \frac{\pi^4}{80}\left(\frac{kT}{\varepsilon_F}\right)^4\right], \tag{17.83′}$$

   and

$$\frac{U}{N} = \frac{3}{5}\varepsilon_F \left[1 + \frac{5\pi^2}{12}\left(\frac{kT}{\varepsilon_F}\right)^2 - \frac{\pi^4}{16}\left(\frac{kT}{\varepsilon_F}\right)^4\right]. \tag{17.84′}$$

   Determine also the T^3-term correction of the specific heat.

8. Plot the energy spectra for the cosmic microwave background at 2.73 K, and for the cosmic neutrino background at 1.95 K.

[3] Pathria 1996, p. 164.

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18 General Relativity

Guided by simple postulates, relativity is a particularly elegant and profound physical theory. Comprehension of general relativity requires a knowledge of the geometry of curved space, a subject with which many physicists are unfamiliar. Maple provides a `tensor` package that greatly facilitates calculations of this kind. With this package, one can obtained geometrical properties necessary in general relativity without knowing details of tensor analysis. On this basis we outline the formulation of relativity, and illustrate some most useful solutions with fascinating applications, such as the Global Positioning System, planetary motion near a black hole and the evolution of the universe.

18.1 Basic Formulation

John Wheeler summarized general relativity in nontechnical terms as "geometry tells matter how to move, and matter tells geometry how to curve."[1] We elaborate this statement by mathematical formulas, and use Maple to bridge the gap between principles and technical details.

The properties of space are described by a *metric*. In three-dimensional Euclidean space, the metric is the square of the infinitesimal separation between two points:

$$dl^2 = dx^2 + dy^2 + dz^2. \tag{18.1}$$

We can express this line element dl in alternative coordinates, such as spherical coordinates r, θ and ϕ:

$$dl^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2. \tag{18.2}$$

From special relativity, we learn that space and time are inseparable: three spatial dimensions and one temporal dimension form a four-dimensional space–time, or the Minkowski space. The square of the space–time interval between a pair of events x^μ and $x^\mu + dx^\mu$ (where the Greek index μ runs from 0 to 3) forms the metric in special relativity:

$$-ds^2 = -c^2dt^2 + dx^2 + dy^2 + dz^2 \equiv -(dx^0)^2 + (dx^1)^2 + (dx^2)^2 + (dx^3)^2. \tag{18.3}$$

[1] Misner, Thorne, and Wheeler 1973, p. 130.

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Avoid any confusion over superscripts on coordinates, which are indices: see equation (12.3). In general relativity this interval is extended to an arbitrary coordinate system,

$$-ds^2 = -c^2 dt^2 + dl^2 = g_{\mu\nu}\, dx^\mu\, dx^\nu, \tag{18.4}$$

which is a quadratic form in differentials of coordinates. In this equation, and hereafter, we invoke the Einstein summation convention introduced in Section 12.1: whenever a Greek index is repeated in a term, summation over this index from 0 to 3 is implied. We note that $g_{\mu\nu}$ is the *metric tensor* introduced in special relativity; a convention $g_{\mu\nu} = \mathrm{diag}(-1, 1, 1, 1)$ corresponds to the Minkowski space. In general relativity, $g_{\mu\nu}$ depends on position; for example, in spherical coordinates the metric is

$$-ds^2 = -c^2 dt^2 + dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2. \tag{18.5}$$

We label the coordinates as

$$x^0 = ct, \quad x^1 = r, \quad x^2 = \theta, \quad x^3 = \phi, \tag{18.6}$$

and identify components of the metric tensor as

$$g_{00} = -1, \quad g_{11} = 1, \quad g_{22} = r^2, \quad g_{33} = r^2 \sin^2\theta, \tag{18.7}$$

and all off-diagonal components vanish. Matrix representation of a tensor of higher rank is impractical; we utilize the Einstein summation notation and express all formulas in components.

The inverse of $g_{\mu\nu}$ is denoted by $g^{\mu\nu}$; together they satisfy a relation

$$g_{\mu\lambda} g^{\lambda\nu} = \delta^\nu_\mu, \tag{18.8}$$

where δ^ν_μ is the Kronecker delta. Extending the nomenclature introduced in Section 12.1, $g_{\mu\nu}$ is a *covariant* tensor of the second rank, having two subscripts as indices; similarly $g^{\mu\nu}$ is a *contravariant* tensor of the second rank, having two superscripts as indices. The Kronecker delta is a *mixed* tensor of the second rank, because it contains both subscript and superscript as indices.

In Chapter 3, we derive the equation of the shortest path between two points on a spherical surface, called a geodesic, using the principle of least action. Analogously, in a four-dimensional space–time, a geodesic corresponds to the minimal space–time interval:

$$-\delta \int ds = 0. \tag{18.9}$$

Recall that ds measures the proper time: $ds = c\, d\tau$. The techniques of calculus of variations are the same, and the differential equations describing equations of motion are obtainable on employing the Euler–Lagrange equation, of which we omit the derivation. It is convenient to express the geodesic equation in terms of the Christoffel symbols, defined as

$$\Gamma^\mu_{\alpha\beta} = \frac{1}{2} g^{\mu\nu} \left(\frac{\partial g_{\alpha\nu}}{\partial x^\beta} + \frac{\partial g_{\beta\nu}}{\partial x^\alpha} - \frac{\partial g_{\alpha\beta}}{\partial x^\nu} \right); \tag{18.10}$$

the condition $\delta \int ds = 0$ results in

$$\frac{d^2x^\mu}{d\tau^2} + \Gamma^\mu_{\nu\lambda}\frac{dx^\nu}{d\tau}\frac{dx^\lambda}{d\tau} = 0. \tag{18.11}$$

Christoffel symbols do not form a tensor, so they cannot have an intrinsic geometrical meaning, or appear in equations of basic physical laws. According to geometry in curved space, the Riemann curvature tensor represents the intrinsic property of space:

$$R^\mu_{\nu\alpha\beta} = \frac{\partial\Gamma^\mu_{\nu\beta}}{\partial x^\alpha} - \frac{\partial\Gamma^\mu_{\nu\alpha}}{\partial x^\beta} + \Gamma^\mu_{\sigma\alpha}\Gamma^\sigma_{\nu\beta} - \Gamma^\mu_{\sigma\beta}\Gamma^\sigma_{\nu\alpha}. \tag{18.12}$$

The importance of the Riemann curvature tensor is that $R^\mu_{\nu\alpha\beta} = 0$ *if and only if* the space is flat. The fourth-rank Riemann tensor becomes "contracted" (through summation of a covariant and a contravariant index) to the Ricci tensor, which is

$$R_{\mu\nu} = R^\sigma_{\mu\nu\sigma}, \tag{18.13}$$

and further to the Ricci scalar,

$$\mathcal{R} = g^{\mu\nu}R_{\mu\nu}. \tag{18.14}$$

Because these definitions are not universally agreed, various signs arise according to which convention is adopted at various stages. The contraction that we employ is consistent with Maple's practice.

The Einstein tensor is defined as

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathcal{R}. \tag{18.15}$$

Both momentum and energy contribute as the source of the gravitational field. The Einstein field equation is

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}\mathcal{R} = -\frac{8\pi G}{c^4}T_{\mu\nu}, \tag{18.16}$$

where $T_{\mu\nu}$ is the energy-momentum tensor; G is the gravitational constant, distinct from the symbol for the Einstein tensor.

The energy-momentum tensor is constructed from the four-velocity dx^μ/ds, energy density $\mathcal{E}$ and the pressure P,

$$T_{\mu\nu} = (P + \mathcal{E})\frac{dx_\mu}{ds}\frac{dx_\nu}{ds} + Pg_{\mu\nu}. \tag{18.17}$$

Although this definition might vary among authors, the quantity T_{00}, which is the energy density, is always positive.

We can lower the index of a contravariant four-vector using the metric tensor:

$$x_\mu = g_{\mu\nu}x^\nu. \tag{18.18}$$

Analogously we can raise an index of a covariant tensor

$$S^{\alpha}_{\beta} = g^{\alpha\mu} S_{\mu\beta}, \tag{18.19}$$

to form a mixed tensor. To eliminate $g_{\mu\nu}$ from the Einstein field equation, because of the prospectively conflicting definition, we express the mixed components of the energy-momentum tensor as

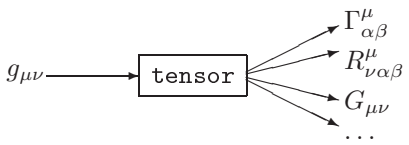
$$T^{\nu}_{\mu} = (P + \mathcal{E}) \frac{dx_\mu}{ds} \frac{dx^\nu}{ds} + P\delta^{\nu}_{\mu}. \tag{18.20}$$

The Einstein field equation in mixed components is then

$$R^{\nu}_{\mu} - \frac{1}{2}\delta^{\nu}_{\mu}\mathcal{R} = -\frac{8\pi G}{c^4} T^{\nu}_{\mu}. \tag{18.21}$$

The left-hand side of the equation is the Einstein tensor, which we write in terms of the Ricci tensor and Ricci scalar to avoid confusion between the Einstein tensor $G_{\mu\nu}$ and gravitational constant G.

To summarize general relativity, "geometry tells matter how to move" means that an object moves such that its proper time between two end conditions is a maximum,[2] or explicitly the geodesic equation (18.11), and "matter tells geometry how to curve" means that matter is the source of the curvature described by the Einstein field equation (18.21). In theory, if we are given an energy distribution, we find the curvature from the Einstein equation, and extract the metric tensor $g_{\mu\nu}$. Knowing the metric, we determine the particle motion. In practice, the Einstein field equation comprises coupled nonlinear differential equations, for which only few exact solutions exist. For the remainder of this chapter, we discuss three of the best known metrics, from which we can learn much about general relativity. Maple is extremely helpful: once we have the metric tensor $g_{\mu\nu}$, there exist explicit formulas, specifically equations (18.10), (18.12), (18.13) and (18.14) ($g_{\mu\nu} \to \Gamma^{\mu}_{\alpha\beta} \to R^{\mu}_{\nu\alpha\beta} \to R_{\mu\nu} \to \mathcal{R}$), which involve first and second partial derivatives with respect to coordinates x^μ, for the Ricci tensor $R_{\mu\nu}$ and Ricci scalar $\mathcal{R}$. Even though symmetry conditions reduce the number of independent components of the Riemann curvature tensor from $4^4 = 256$ to 20, the calculation is considerable; such a tedious but straightforward task is certainly the ultimate strength of computer algebra.



[2] Because $-\int ds$ is a minimum, $c\int d\tau = \int ds$ is a maximum.

18.2 Newtonian Limit

The square of the space–time interval that is associated with a weak field takes this form,

$$-ds^2 = -\left(1+\frac{2\Phi}{c^2}\right)c^2dt^2 + \left(1-\frac{2\Phi}{c^2}\right)(dx^2+dy^2+dz^2), \tag{18.22}$$

where Φ is the gravitational potential. We use this metric as an example to illustrate how to obtain the Einstein tensor using Maple. Many authors set the speed of light c to unity to simplify the expression, but we maintain c explicitly in this chapter so that we can use Maple to find the corresponding Newtonian limit by setting c to infinity. In the limit of $\Phi/c^2 \ll 1$, this space–time interval reduces to that of the Minkowski space. If we define our coordinates in the Minkowski space as

$$x^\mu = (t, x, y, z), \tag{18.23}$$

we can absorb c in the metric,

$$g_{\mu\nu} = \text{diag}(-c^2, 1, 1, 1).$$

With this assignment, we have

$$x_\mu = g_{\mu\nu}x^\nu = (-c^2t, x, y, z).$$

It is convenient to use this definition of coordinates and metric tensor in Maple; later on we can avoid $g_{\mu\nu}$ in the field equation by expressing the Einstein tensor in mixed rank.

Returning our attention to the weak field, we identify the metric tensor as

$$g_{\mu\nu} = \text{diag}\left(-c^2-2\Phi, 1-\frac{2\Phi}{c^2}, 1-\frac{2\Phi}{c^2}, 1-\frac{2\Phi}{c^2}\right). \tag{18.24}$$

Once we provide the metric, Maple calculates the Christoffel symbols and the Riemann tensor directly from equations (18.10), (18.12), (18.13) and (18.14).

Worksheet 18.1 This worksheet, which is a modification of an example in Maple's help files under `tensor`, serves as a satisfactory template for most relativity calculations. Given $g_{\mu\nu}$, the `tensor` package implements the entire calculation with the `tensorsGR` command. One needs to supply the coordinates (denoted `coords` in our example) and the metric tensor (`metric`), and `tensorsGR` returns the rest 9 arguments such as $\Gamma^\mu_{\alpha\beta}$ and $G_{\mu\nu}$. To conform to Maple's notation, we adjust the index to run from 1 to 4, instead of from 0 to 3 discussed in the text; be aware of this shift. The index character (`index_char`), having values -1 or $+1$, specifies an index as covariant (subscript) or contravariant (superscript), respectively. Because Maple returns the Einstein tensor (`GEin`) as a covariant tensor (having index character `[-1,-1]`), to produce a mixed-rank tensor, we use the contravariant metric tensor $g^{\mu\nu}$ (denoted `contra_metric`), and the `raise` command.

```
> with(tensor):
> coords := [t, x, y, z]:
> g := array(symmetric, sparse, 1..4, 1..4):
> g[1,1] := -c^2 - 2*Phi(x,y,z):  g[2,2] := 1 - 2*Phi(x,y,z)/c^2:
> g[3,3] := g[2,2]:  g[4,4] := g[2,2]:  metric := create([-1,-1],
> eval(g));
```

$$metric := \mathrm{table}([compts$$

$$= \begin{bmatrix} -c^2 - 2\,\Phi(x,\,y,\,z) & 0 & 0 & 0 \\ 0 & 1 - \dfrac{2\,\Phi(x,\,y,\,z)}{c^2} & 0 & 0 \\ 0 & 0 & 1 - \dfrac{2\,\Phi(x,\,y,\,z)}{c^2} & 0 \\ 0 & 0 & 0 & 1 - \dfrac{2\,\Phi(x,\,y,\,z)}{c^2} \end{bmatrix},$$

$$index_char = [-1,\,-1]$$

$$])$$

```
> tensorsGR(coords, metric, contra_metric, det_met, C1, C2, Rm, Rc,
> R, GEin, C):
> rGEin := raise(contra_metric, GEin, 1):
> comp_rGEin := get_compts(rGEin):
> comp_rGEin[1,1];
```

$$\begin{aligned} &c^2(2\,(\tfrac{\partial^2}{\partial y^2}\,\Phi(x,\,y,\,z))\,c^2 + 2\,(\tfrac{\partial^2}{\partial x^2}\,\Phi(x,\,y,\,z))\,c^2 + 2\,(\tfrac{\partial^2}{\partial z^2}\,\Phi(x,\,y,\,z))\,c^2 \\ &+3\,(\tfrac{\partial}{\partial x}\,\Phi(x,\,y,\,z))^2 + 3\,(\tfrac{\partial}{\partial z}\,\Phi(x,\,y,\,z))^2 + 3\,(\tfrac{\partial}{\partial y}\,\Phi(x,\,y,\,z))^2 \\ &-4\,(\tfrac{\partial^2}{\partial x^2}\,\Phi(x,\,y,\,z))\,\Phi(x,\,y,\,z) - 4\,(\tfrac{\partial^2}{\partial y^2}\,\Phi(x,\,y,\,z))\,\Phi(x,\,y,\,z) \\ &-4\,(\tfrac{\partial^2}{\partial z^2}\,\Phi(x,\,y,\,z))\,\Phi(x,\,y,\,z))\Big/(c^2 - 2\,\Phi(x,\,y,\,z))^3 \end{aligned}$$

```
> limit(comp_rGEin[1,1]*c^2, c=infinity);
```

$$2\,(\tfrac{\partial^2}{\partial y^2}\,\Phi(x,\,y,\,z)) + 2\,(\tfrac{\partial^2}{\partial x^2}\,\Phi(x,\,y,\,z)) + 2\,(\tfrac{\partial^2}{\partial z^2}\,\Phi(x,\,y,\,z))$$

We omit listing all components of the Einstein tensor, but restrict our attention to the 0-0 component. We are interested in the limit $c^2 \gg \Phi$:

$$\lim_{c\to\infty} c^2 G_0^0 = 2\left(\frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} + \frac{\partial^2\Phi}{\partial z^2}\right) = 2\,\nabla^2\Phi. \tag{18.25}$$

The energy density $\mathcal{E}$ is related to the mass density ρ as $\mathcal{E} = \rho c^2$, thus $T_0^0 = -\rho c^2$; substituting

this into the Einstein field equation, we have the 0-0 component:

$$G_0^0 = -\frac{8\pi G}{c^4} T_0^0, \quad \frac{2}{c^2}\nabla^2\Phi = \frac{8\pi G}{c^4}\rho c^2; \tag{18.26}$$

distinguish G_0^0, which is the temporal component of the Einstein tensor, from G, the gravitational constant. The above equation is none other than the Poisson equation:

$$\nabla^2\Phi = 4\pi G\rho, \tag{18.27}$$

which is Newton's law of gravitation.

18.2.1 Gravitational Redshift

The Poisson equation is well studied in electromagnetism. From the solution of the electric potential, we can directly write the solution of equation (18.27) as

$$\Phi = -\int \frac{G\rho(\mathbf{r}_2)}{r_{12}}\, dV_2. \tag{18.28}$$

In particular, outside a spherical object of mass M, the potential is

$$\Phi = -\frac{GM}{r}. \tag{18.29}$$

The metric equation (18.22) yields the proper time τ, when the spatial components vanish:

$$d\tau = \left(1 - \frac{2GM}{rc^2}\right)^{1/2} dt \cong \left(1 - \frac{GM}{rc^2}\right) dt. \tag{18.30}$$

This equation indicates the gravitational redshift: as a clock runs more slowly in a gravitational field than in its absence, time elapsed in the absence of a gravitational field, dt, is always greater than that in a gravitational field, $d\tau$.

Example 18.1 Consider a satellite that orbits the earth on a circular path with a period of 12 hours; this configuration resembles that of the Global Positioning System. Evaluate the discrepancy of time between one clock on this satellite and another on the equator on earth, due to both special and general relativity, after one day of operation. The reference is a clock at the geocenter, for which one assumes no motion and no gravitational field.

Solution Knowing the period of the satellite, we can calculate the orbiting radius and the velocity from Newtonian mechanics as an approximation. For circular motion with a force according to the inverse-square law,

$$\frac{GMm}{r^2} = m\omega^2 r, \tag{18.31}$$

where

$$\omega = \frac{2\pi}{T};$$

thus we obtain the radius and velocity of the satellite:

$$r_{\text{sat}} = \frac{(GM)^{1/3}}{\omega_{\text{sat}}^{2/3}}, \quad v_{\text{sat}} = \omega_{\text{sat}} r_{\text{sat}}. \tag{18.32}$$

Knowing the radius of the earth r_{earth}, we calculate the velocity on the equator to be

$$v_{\text{earth}} = \omega_{\text{earth}} r_{\text{earth}}. \tag{18.33}$$

In addition to the effect of gravitational redshift which appears in equation (18.30), the effect of dilation of time due to the motion of the clocks must be considered as well. Because $ds = c\,d\tau$, from equation (18.22) we derive

$$d\tau = \sqrt{1 - \frac{2GM}{rc^2} - \frac{v^2}{c^2}}\, dt. \tag{18.34}$$

Note that in the absence of M, this equation becomes

$$d\tau = \sqrt{1 - \frac{v^2}{c^2}}\, dt,$$

a familiar result in special relativity.

In sum, the time difference is

$$\Delta\tau_{\text{sat}} - \Delta\tau_{\text{earth}} = \left(\sqrt{1 - \frac{2GM}{r_{\text{sat}}c^2} - \frac{v_{\text{sat}}^2}{c^2}} - \sqrt{1 - \frac{2GM}{r_{\text{earth}}c^2} - \frac{v_{\text{earth}}^2}{c^2}} \right) \Delta t. \tag{18.35}$$

We have all the information required concerning the radius and the velocity.

Worksheet 18.2 This worksheet involves only basic algebra. Because the relativistic modification is typically small, to ensure sufficient precision we use the command `Digits := n`, which serves to calculate and to display subsequent answers with n digits.

```
> Eq1 := G*M*m/r^2 = m*w^2*r;
```

$$Eq1 := \frac{G\,M\,m}{r^2} = m\,w^2\,r$$

```
> Soln1 := solve(Eq1, r);
```

$$Soln1 := \frac{(G\,M\,w)^{(1/3)}}{w}, -\frac{(G\,M\,w)^{(1/3)}}{2\,w} + \frac{\frac{1}{2}\,I\,\sqrt{3}\,(G\,M\,w)^{(1/3)}}{w},$$
$$-\frac{(G\,M\,w)^{(1/3)}}{2\,w} - \frac{\frac{1}{2}\,I\,\sqrt{3}\,(G\,M\,w)^{(1/3)}}{w}$$

```
> rsat := Soln1[1];
```

$$rsat := \frac{(G\,M\,w)^{(1/3)}}{w}$$

```
> G:=6.673e-11; c:=299792458; M:=5.974e24; rearth:=6.38e6;
```

$$G := 0.6673\,10^{-10}$$
$$c := 299792458$$
$$M := 0.5974\,10^{25}$$
$$rearth := 0.638\,10^{7}$$

```
> Tsat := 12*60*60; Tearth := 24*60*60;
```

$$Tsat := 43200$$
$$Tearth := 86400$$

```
> wsat := 2*Pi/Tsat:
> rsat := eval(rsat,w=wsat):
> rsat := evalf(rsat);
```

$$rsat := 0.2661121476\,10^{8}$$

```
> vsat := wsat*rsat:
> vsat := evalf(vsat);
```

$$vsat := 3870.444295$$

```
> vearth := 2*Pi*rearth/Tearth:
> vearth := evalf(vearth);
```

$$vearth := 463.9666929$$

```
> Digits := 20:
> tdf := (sqrt((1 - 2*G*M/(rsat*c^2)) - (vsat/c)^2) - sqrt((1 -
> 2*G*M/(rearth*c^2)) - (vearth/c)^2))*Tearth;
```

$$tdf := 0.00003856918904294400$$

This calculation indicates that the difference between times on a clock on the satellite and on a clock on earth is $38.6\ \mu$s each day, with the clock on earth running more slowly. It is necessary to calibrate a clock carried by a satellite so that it remains synchronized with a clock on earth. We leave it to the reader to discern that general relativity makes a greater contribution to this difference than does special relativity.

18.3 Schwarzschild Solution

As mentioned earlier, the Einstein equation consists of a system of coupled nonlinear partial differential equations, and there are no general methods for obtaining the solutions. Indeed, very few solutions of physical interest have been found; among them, the Schwarzschild so-

lution is perhaps the most useful one:

$$-ds^2 = -\left(c^2 - \frac{2GM}{r}\right) dt^2 + \frac{dr^2}{1 - \dfrac{2GM}{c^2 r}} - r^2(d\theta^2 + \sin^2\theta d\phi^2). \tag{18.36}$$

This solution represents the exterior of a spherically symmetric gravitational source M. The Schwarzschild solution facilitates the treatment of the two-body problem in general relativity. In this section, we first use Maple to calculate the Christoffel symbols so that we obtain the geodesics; as an alternative, we employ the techniques developed in our discussion of the Lagrangian formulation of mechanics to find the trajectory of a particle near a compact object such as a neutron star or a black hole.

The metric tensor is

$$g_{\mu\nu} = \text{diag}\left[-c^2 + \frac{2GM}{r}, \left(1 - \frac{2GM}{cr^2}\right)^{-1}, r^2, r^2\sin^2\theta\right], \tag{18.37}$$

with spherical coordinates

$$x^\mu = (t, r, \theta, \phi)\,. \tag{18.38}$$

We first evaluate the Christoffel symbols, which are defined in equation (18.10), and then the geodesic, equation (18.11); `tensor` accomplishes all of this task.

Worksheet 18.3 We simply modify the worksheet in the preceding section, by supplying `g` and `coords` corresponding to the Schwarzschild metric.

```
> with(tensor):
> coords:=[t, r, theta,phi]:
> g := array(symmetric, sparse, 1..4, 1..4):
> g[1,1] := -(c^2 - 2*G*m/r):  g[2,2] := -c^2/g[1,1]:
> g[3,3] := r^2:  g[4,4] := r^2*sin(theta)^2:
> metric := create([-1,-1], eval(g));
```

$$metric := \text{table}([index_char = [-1, -1],$$

$$compts = \begin{bmatrix} -c^2 + \dfrac{2\,G\,m}{r} & 0 & 0 & 0 \\ 0 & -\dfrac{c^2}{-c^2 + \dfrac{2\,G\,m}{r}} & 0 & 0 \\ 0 & 0 & r^2 & 0 \\ 0 & 0 & 0 & r^2\sin(\theta)^2 \end{bmatrix}$$

$$])$$

```
> tensorsGR(coords, metric, contra_metric, det_met, C1, C2, Rm, Rc,
> R, GE, C):
> displayGR(Christoffel2, C2);
```

The Christoffel Symbols of the Second Kind

$$non - zero\ components\ :$$

$$\{1, 12\} = \frac{G\,m}{r\,(c^2\,r - 2\,G\,m)}$$

$$\{2, 11\} = \frac{(c^2\,r - 2\,G\,m)\,G\,m}{c^2\,r^3}$$

$$\{2, 22\} = -\frac{G\,m}{r\,(c^2\,r - 2\,G\,m)}$$

$$\{2, 33\} = -\frac{c^2\,r - 2\,G\,m}{c^2}$$

$$\{2, 44\} = -\frac{(c^2\,r - 2\,G\,m)\sin(\theta)^2}{c^2}$$

$$\{3, 23\} = \frac{1}{r}$$

$$\{3, 44\} = -\sin(\theta)\cos(\theta)$$

$$\{4, 24\} = \frac{1}{r}$$

$$\{4, 34\} = \frac{\cos(\theta)}{\sin(\theta)}$$

```
> Eqns := geodesic_eqns(coords, s, C2 );
```

$$Eqns := \left\{ (\tfrac{d^2}{ds^2}\,\phi(s)) + \frac{2\,(\frac{d}{ds}\,\mathrm{r}(s))\,(\frac{d}{ds}\,\phi(s))}{r} + \frac{2\cos(\theta)\,(\frac{d}{ds}\,\theta(s))\,(\frac{d}{ds}\,\phi(s))}{\sin(\theta)} = 0,\right.$$

$$(\tfrac{d^2}{ds^2}\,\mathrm{r}(s)) + \frac{(c^2\,r - 2\,G\,m)\,G\,m\,(\frac{d}{ds}\,\mathrm{t}(s))^2}{c^2\,r^3} - \frac{G\,m\,(\frac{d}{ds}\,\mathrm{r}(s))^2}{r\,(c^2\,r - 2\,G\,m)}$$

$$-\frac{(c^2\,r - 2\,G\,m)\,(\frac{d}{ds}\,\theta(s))^2}{c^2} - \frac{(c^2\,r - 2\,G\,m)\sin(\theta)^2\,(\frac{d}{ds}\,\phi(s))^2}{c^2} = 0,$$

$$(\tfrac{d^2}{ds^2}\,\theta(s)) + \frac{2\,(\frac{d}{ds}\,\mathrm{r}(s))\,(\frac{d}{ds}\,\theta(s))}{r} - \sin(\theta)\cos(\theta)\,(\tfrac{d}{ds}\,\phi(s))^2 = 0,$$

$$\left.(\tfrac{d^2}{ds^2}\,\mathrm{t}(s)) + \frac{2\,G\,m\,(\frac{d}{ds}\,\mathrm{t}(s))\,(\frac{d}{ds}\,\mathrm{r}(s))}{r\,(c^2\,r - 2\,G\,m)} = 0\right\}$$

According to our notation, the Christoffel symbols are

$$\Gamma^t_{tr} = \frac{GM}{r^2}\frac{1}{c^2 - \frac{2GM}{r}},$$

$$\Gamma^r_{tt} = \frac{GM}{c^2 r^4}\left(c^2 - \frac{2GM}{r}\right), \quad \Gamma^r_{rr} = -\frac{GM}{r^2}\frac{1}{c^2 - \frac{2GM}{r}},$$

$$\Gamma^r_{\theta\theta} = -\frac{r}{c^2}\left(c^2 - \frac{2GM}{r}\right), \quad \Gamma^r_{\phi\phi} = -\frac{r}{c^2}\left(c^2 - \frac{2GM}{r}\right)\sin^2\theta,$$

$$\Gamma^\theta_{r\theta} = \frac{1}{r}, \quad \Gamma^\theta_{\phi\phi} = -\sin\theta\cos\theta,$$

$$\Gamma^\phi_{r\phi} = \frac{1}{r}, \quad \Gamma^\phi_{\theta\phi} = \cot\theta, \tag{18.39}$$

where we use t, r, θ and ϕ as indices instead of 0, 1, 2 and 3. We let the reader list components of the Riemann curvature tensor $R^\mu_{\nu\alpha\beta}$ and of the Ricci tensor $R_{\mu\nu}$; the latter can be considered the average curvature, which is zero even though there are nonvanishing $R^\mu_{\nu\alpha\beta}$.

The geodesic equations are

$$\frac{d^2\theta}{ds^2} + \frac{2}{r}\frac{dr}{ds}\frac{d\theta}{ds} - \sin\theta\cos\theta\left(\frac{d\phi}{ds}\right)^2 = 0, \tag{18.40a}$$

$$\frac{d^2\phi}{ds^2} + \frac{2}{r}\frac{dr}{ds}\frac{d\phi}{ds} + 2\cot\theta\frac{d\theta}{ds}\frac{d\phi}{ds} = 0, \tag{18.40b}$$

$$\frac{d^2t}{ds^2} + \frac{2GM}{r^2}\frac{1}{c^2 - \frac{2GM}{r}}\frac{dt}{ds}\frac{dr}{ds} = 0, \tag{18.40c}$$

$$\frac{d^2r}{ds^2} + \frac{c^2 - \frac{2GM}{r}}{c^2}\frac{GM}{r^2}\left(\frac{dt}{ds}\right)^2 - \frac{1}{c^2 - \frac{2GM}{r}}\frac{GM}{r^2}\left(\frac{dr}{ds}\right)^2 - \frac{c^2 - \frac{2GM}{r}}{c^2}r\left(\frac{d\theta}{ds}\right)^2 - \frac{c^2 - \frac{2GM}{r}}{c^2}r\sin^2\theta\left(\frac{d\phi}{ds}\right)^2 = 0. \tag{18.40d}$$

Although these equations appear complicated, with given initial conditions we can numerically solve these four differential equations to obtain the trajectory. Analogously to the method used for the Kepler problem, we make some rearrangement of these equations to decouple them. Because it is inconvenient to manipulate equations from the output of the `tensor` package, as they arise in a form not directly amenable to application of the `dsolve` command, we apply instead the method developed in Chapter 3 to obtain geodesic equations directly from the metric, using the principle of least action.

To simplify the problem, we solve equation (18.40a). If at one instant $\theta = \pi/2$, then

$$\left.\frac{d\theta}{ds}\right|_0 = 0, \quad \cos\theta|_0 = 0, \quad \left.\frac{d^2\theta}{ds^2}\right|_0 = 0;$$

thus θ remains constant, which confines particle motion to the same plane.

For a constant value $\theta = \pi/2$, the metric becomes

$$-ds^2 = -\left(c^2 - \frac{2GM}{r}\right) dt^2 + \frac{dr^2}{1 - \dfrac{2GM}{c^2 r}} + r^2 d\phi^2. \tag{18.41}$$

The geodesic equation specifies a path that minimizes the integral of ds, for which it is equivalent to find functions that make

$$\delta \int \frac{ds^2}{2} = 0.$$

We let s be the independent variable, and t, r, and ϕ dependent variables; hence

$$-ds^2 = \left[-\left(c^2 - \frac{2GM}{r}\right) \left(\frac{dt}{ds}\right)^2 + \frac{1}{1 - \dfrac{2GM}{c^2 r}} \left(\frac{dr}{ds}\right)^2 + r^2 \left(\frac{d\phi}{ds}\right)^2 \right] ds^2.$$

We apply the Euler–Lagrange equation to function f, identified as

$$f = \frac{1}{2} \left[-\left(c^2 - \frac{2GM}{r}\right) \left(\frac{dt}{ds}\right)^2 + \frac{1}{1 - \dfrac{2GM}{c^2 r}} \left(\frac{dr}{ds}\right)^2 + r^2 \left(\frac{d\phi}{ds}\right)^2 \right],$$

to obtain the equations of motion; this function is the Lagrangian for the Schwarzschild solution.

For the t and ϕ coordinates, because f contains no explicit dependence on t and ϕ, we exploit the symmetry property by introducing two constants a and h,

$$\frac{\partial f}{\partial \left(\frac{dt}{ds}\right)} = -\frac{a}{c}, \quad \left(c^2 - \frac{2GM}{r}\right) \frac{dt}{ds} = \frac{a}{c},$$

and

$$\frac{\partial f}{\partial \left(\frac{d\phi}{ds}\right)} = \frac{h}{c}, \quad r^2 \frac{d\phi}{ds} = \frac{h}{c}.$$

For the r coordinate,

$$\frac{d}{ds} \frac{\partial f}{\partial \left(\frac{dr}{ds}\right)} - \frac{\partial f}{\partial r} = 0,$$

$$\frac{1}{1 - \frac{2GM}{c^2 r}} \frac{d^2 r}{ds^2} - r \left(\frac{d\phi}{ds}\right)^2 + \left[\left(\frac{dt}{ds}\right)^2 - \frac{1}{\left(1 - \frac{2GM}{c^2 r}\right)^2} \frac{1}{c^2} \left(\frac{dr}{ds}\right)^2 \right] \frac{GM}{r^2} = 0.$$

To rearrange the above three equations, we first isolate dt/ds and $d\phi/ds$,

$$\frac{d\phi}{ds} = \frac{1}{c}\frac{h}{r^2}, \tag{18.42}$$

$$\frac{dt}{ds} = \frac{1}{c}\frac{a}{c^2 - \frac{2GM}{r}}. \tag{18.43}$$

We then decouple the r equation:

$$c^2\frac{d^2r}{ds^2} - \left(1 - \frac{2GM}{c^2r}\right)\frac{h^2}{r^3} + \left[\frac{a^2}{c^4} - \left(\frac{dr}{ds}\right)^2\right]\frac{1}{1 - \frac{2GM}{c^2r}}\frac{GM}{r^2} = 0. \tag{18.44}$$

Equation (18.42) resembles Kepler's law in classical mechanics; the constant h that we introduce corresponds to the angular momentum per unit mass. We list equations (4.20) and (4.21) of the classical Kepler problem for comparison,

$$\frac{d\phi}{dt} = \frac{\tilde{l}}{r^2},$$

$$\frac{d^2r}{dt^2} - \frac{\tilde{l}^2}{r^3} + \frac{GM}{r^2} = 0,$$

where $\tilde{l}$ is the angular momentum per unit mass, l/m.

Just as for the Kepler problem before, we can numerically solve equations (18.42) and (18.44). To compare our result with the literature, we invoke additional information about the energy, although to find the trajectory of a particle, such knowledge is not required. Because the metric has no dependence on time, the energy of the system is conserved, which is related to the constant a that we assigned. According to *Gravitation* by Misner et al. 1973, p. 660, this constant a that we introduced corresponds to the energy per unit mass,

$$\frac{a^2}{c^4} = \left(\frac{dr}{ds}\right)^2 + \frac{\tilde{V}^2}{c^4}, \tag{18.45a}$$

where

$$\frac{\tilde{V}^2}{c^4} = \left(1 - \frac{2GM}{c^2r}\right)\left(1 + \frac{h^2}{c^2r^2}\right). \tag{18.45b}$$

This equation arises from the fact that the scalar product of four-velocity with itself is an invariant. We generally refer to $\tilde{V}$ as the "effective potential." A plot of the effective potential allows us to examine the range of radial motion, and to determine turning points, at which $a = \tilde{V}$.

Worksheet 18.4 The technique of employing the Euler–Lagrange equation is extensively discussed in Chapter 4. The equations of motion of the t, r and ϕ coordinates are `Eq14`, `Eq26` and `Eq34`, respectively. The algebraic manipulation to decouple differential equations are the same as the Kepler problem in Chapter 4. We set G and c equal to unity, and assign

initial values r_0, $\dot{r}_0$, ϕ_0 and $\dot{\phi}_0$; thus we can calculate the angular momentum h and the energy a (both per unit mass). We solve two differential equations, namely `Eq54` and `Eq55`, numerically. For reference, a plot of the effective potential and total energy is included. The `dsolve` and `polarplot` commands apply in the same way as for the Kepler problem.

```
> f := 1/2*(-(c^2 - 2*G*M/r(s))*diff(t(s),s)^2 +
> 1/(1 - 2*G*M/(c^2*r(s)))*diff(r(s),s)^2 +
r(s)^2*diff(phi(s),s)^2);
```

$$f := -\frac{1}{2}\left(c^2 - \frac{2\,G\,M}{\mathrm{r}(s)}\right)\left(\tfrac{d}{ds}\,\mathrm{t}(s)\right)^2 + \frac{1}{2}\,\frac{\left(\tfrac{d}{ds}\,\mathrm{r}(s)\right)^2}{1 - \dfrac{2\,G\,M}{c^2\,\mathrm{r}(s)}} + \frac{1}{2}\,\mathrm{r}(s)^2\left(\tfrac{d}{ds}\,\phi(s)\right)^2$$

```
> f1 := subs({t(s)=var1, diff(t(s),s)=var2, r(s)=var3,
> diff(r(s),s)=var4, phi(s)=var5, diff(phi(s),s)=var6}, f):
> Epr11 := diff(f1, var2):
> Epr12 := diff(f1, var1):
> Epr13 := subs({var1=t(s), var2=diff(t(s),s), var3=r(s),
> var5=phi(s), var4=diff(r(s),s), var6=diff(phi(s),s)}, Epr11):
> Eq14 := Epr13 = -a/c;
```

$$Eq14 := -\left(c^2 - \frac{2\,G\,M}{\mathrm{r}(s)}\right)\left(\tfrac{d}{ds}\,\mathrm{t}(s)\right) = -\frac{a}{c}$$

```
> Epr21 := diff(f1, var4):
> Epr22 := diff(f1, var3):
> Epr23 := subs({var1=t(s), var2=diff(t(s),s), var3=r(s),
> var5=phi(s), var4=diff(r(s),s), var6=diff(phi(s),s)}, Epr21):
> Epr24 := subs({var1=t(s), var2=diff(t(s),s), var3=r(s),
> var5=phi(s), var4=diff(r(s),s), var6=diff(phi(s),s)}, Epr22):
> Epr25 := diff(Epr23, s):
> Eq26 := Epr25 - Epr24 = 0;
```

$$Eq26 := -\frac{\left(\tfrac{d}{ds}\,\mathrm{r}(s)\right)^2 G\,M}{\left(1 - \dfrac{2\,G\,M}{c^2\,\mathrm{r}(s)}\right)^2 c^2\,\mathrm{r}(s)^2} + \frac{\tfrac{d^2}{ds^2}\,\mathrm{r}(s)}{1 - \dfrac{2\,G\,M}{c^2\,\mathrm{r}(s)}} + \frac{G\,M\left(\tfrac{d}{ds}\,\mathrm{t}(s)\right)^2}{\mathrm{r}(s)^2} - \mathrm{r}(s)\left(\tfrac{d}{ds}\,\phi(s)\right)^2 = 0$$

```
> Epr31 := diff(f1, var6):
> Epr32 := diff(f1, var5):
```

```
> Epr33 := subs({var1=t(s), var2=diff(t(s),s), var3=r(s),
> var5=phi(s), var4=diff(r(s),s), var6=diff(phi(s),s)}, Epr31):
> Eq34 := Epr33 = h/c;
```

$$Eq34 := \mathrm{r}(s)^2 \left(\frac{d}{ds}\,\phi(s)\right) = \frac{h}{c}$$

```
> Eq53 := isolate(Eq14, diff(t(s),s));
```

$$Eq53 := \frac{d}{ds}\,\mathrm{t}(s) = -\frac{a}{c\left(-c^2 + \dfrac{2\,G\,M}{\mathrm{r}(s)}\right)}$$

```
> Eq54 := isolate(Eq34, diff(phi(s),s));
```

$$Eq54 := \frac{d}{ds}\,\phi(s) = \frac{h}{c\,\mathrm{r}(s)^2}$$

```
> Eq55 := eval(Eq26, {Eq53, Eq54});
```

$$Eq55 := -\frac{\left(\frac{d}{ds}\,\mathrm{r}(s)\right)^2 G\,M}{\left(1 - \dfrac{2\,G\,M}{c^2\,\mathrm{r}(s)}\right)^2 c^2\,\mathrm{r}(s)^2} + \frac{\frac{d^2}{ds^2}\,\mathrm{r}(s)}{1 - \dfrac{2\,G\,M}{c^2\,\mathrm{r}(s)}} + \frac{G\,M\,a^2}{\mathrm{r}(s)^2\,c^2\left(-c^2 + \dfrac{2\,G\,M}{\mathrm{r}(s)}\right)^2} - \frac{h^2}{\mathrm{r}(s)^3\,c^2} = 0$$

```
> M := 1; G := 1; c := 1;
```

$$M := 1$$
$$G := 1$$
$$c := 1$$

```
> Eq77 := r(0) = 11;
```

$$Eq77 := \mathrm{r}(0) = 11$$

```
> Eq78 := D(r)(0) = 0;
```

$$Eq78 := \mathrm{D}(r)(0) = 0$$

```
> Eq79 := phi(0) = 0;
```

$$Eq79 := \phi(0) = 0$$

```
> Eq80 := D(phi)(0) = 0.0295;
```

$$Eq80 := \mathrm{D}(\phi)(0) = 0.0295$$

```
> h := eval(lhs(Eq34), {r(s)=rhs(Eq77), diff(phi(s),s)=rhs(Eq80)});
```

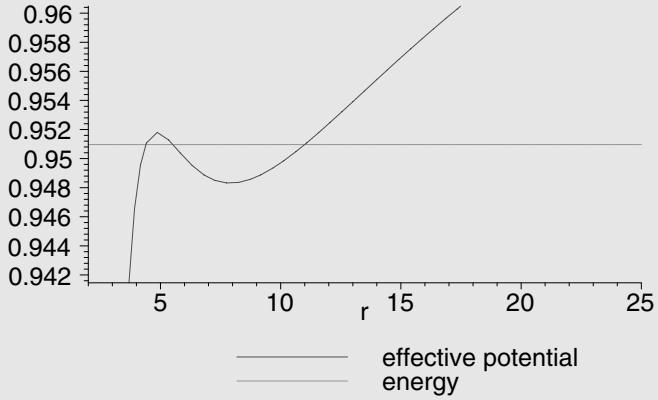
$$h := 3.5695$$

```
> a := sqrt((1 - 2*M/rhs(Eq77))*(1 + h^2/rhs(Eq77)^2));
```

$$a := 0.9509661236$$

```
> Vsq := sqrt((1 - 2*M/x)*(1 + h^2/x^2)):
```

```
> plot([Vsq, a], x=2..25, a-0.01*a..a+0.01*a, legend=["effective
> potential", "energy"]);
```




```
> ini := Eq77, Eq78, Eq79;
```

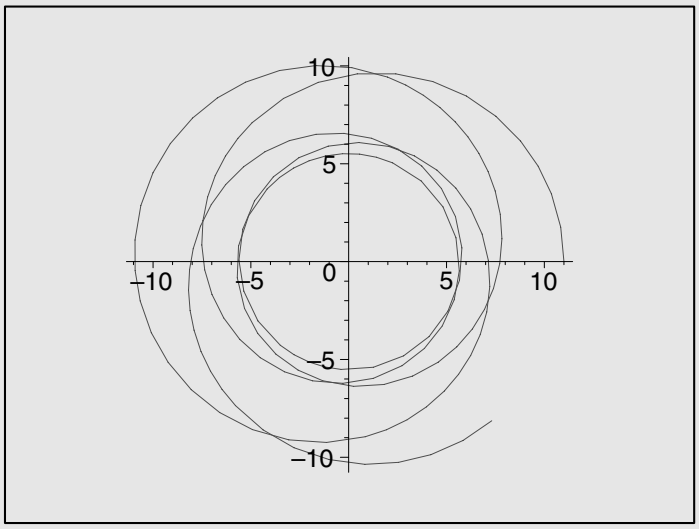
$$ini := \mathrm{r}(0) = 11, \mathrm{D}(r)(0) = 0, \phi(0) = 0$$

```
> Eq91 := dsolve({Eq54, Eq55, ini}, {r(s), phi(s)}, numeric,
> output=listprocedure);
```

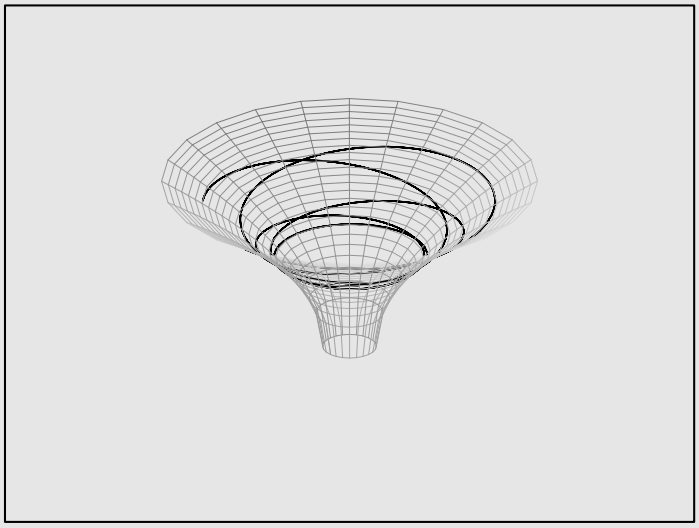
$$Eq91 := [s = (\textbf{proc}(s) \ldots \textbf{end proc}\ ), \phi(s) = (\textbf{proc}(s) \ldots \textbf{end proc}),$$
$$\mathrm{r}(s) = (\textbf{proc}(s) \ldots \textbf{end proc}), \tfrac{d}{ds}\mathrm{r}(s) = (\textbf{proc}(s) \ldots \textbf{end proc})]$$

```
> with(plots):
Warning, the name changecoords has been redefined

> polarplot([rhs(Eq91(s)[3]), rhs(Eq91(s)[2]), s=0..500],
> scaling=constrained);
```




```
> p1 := plot3d([x*cos(t), x*sin(t), sqrt(8*(x-2))], x=2..14,
> t=0..2*Pi, style=hidden):
> p2 := spacecurve([rhs(Eq91(s)[3]), rhs(Eq91(s)[2]),
> sqrt(8*(rhs(Eq91(s)[3])-2)), s=0..500], coords=cylindrical,
> color=black, numpoints=400):
> display([p1, p2]);
```



```
> animate(polarplot, [[rhs(Eq91(s)[3]), rhs(Eq91(s)[2]), s=0..t]],
> t=0..500, scaling=constrained);
```

```
> p3 := animate(spacecurve, [[rhs(Eq91(s)[3]), rhs(Eq91(s)[2]),
> sqrt(8*(rhs(Eq91(s)[3])-2))], s=0..t, coords=cylindrical,
> numpoints=400, color=black], t=0..500):
> display([p1, p3]);
```

From the plot of the effective potential, the particle should be confined in an annular region specified by $5.5M \leq r \leq 11.0M$ (geometrized unit), which we verify from the plot of the trajectory based on numerical solution. We observe a precession of the particle's motion. In general relativity the space is curved. To visualize a curved space, we include an embedding diagram of a slice of the equatorial plane, with depth z to accommodate the actual radial distance, which is greater than the coordinate r by a factor of $(1-2M/r)^{-1/2}$. With $G = c = 1$, the embedding formula for the Schwarzschild metric is

$$z = \sqrt{8M(r-2M)}; \tag{18.46}$$

see Appendix B.5 for a derivation. We also list in the worksheet the code used to implement animation for this motion.

18.4 Robertson–Walker Metric

We introduce a metric that depends on time. On a large scale, our universe is homogeneous and isotropic; the Robertson–Walker metric, on which standard cosmology is based, describes these properties:

$$-ds^2 = -c^2dt^2 + a^2(t)\left(\frac{dr^2}{1-kr^2} + r^2d\theta^2 + r^2\sin^2\theta d\phi^2\right). \tag{18.47}$$

In this metric, the time-dependent parameter $a(t)$ is the cosmic scale factor; the time-independent parameter k determines the intrinsic curvature of space, which can be positive, zero or negative. The metric tensor is

$$g_{\mu\nu} = \text{diag}\left(-c^2, \frac{a^2}{1-kr^2}, a^2r^2, a^2r^2\sin^2\theta\right), \tag{18.48}$$

with coordinates

$$x^\mu = (t, r, \theta, \phi)\,. \tag{18.49}$$

Having Maple perform the calculations, we obtain the Einstein tensor from this metric:

$$G^0_0 = 3\left(\frac{\dot{a}^2}{c^2a^2} + \frac{k}{a^2}\right), \tag{18.50}$$

$$G^1_1 = G^2_2 = G^3_3 = \frac{2\ddot{a}}{c^2a} + \frac{\dot{a}^2}{c^2a^2} + \frac{k}{a^2}. \tag{18.51}$$

Worksheet 18.5 After we provide g and `coords`, Maple evaluates the Einstein tensor; see the worksheet in Section 18.2 for an explanation.

```
> coords := [t, r, theta, phi]:
> g := array(symmetric, sparse, 1..4, 1..4):
> g[1,1] := -c^2:  g[2,2] := (a(t))^2/(1 - k*r^2):
> g[3,3] := (a(t)*r)^2:  g[4,4] := (a(t)*r*sin(theta))^2:
> metric := create([-1,-1], eval(g));
```

$$metric := \mathrm{table}([compts = \begin{bmatrix} -c^2 & 0 & 0 & 0 \\ 0 & \dfrac{\mathrm{a}(t)^2}{1-k\,r^2} & 0 & 0 \\ 0 & 0 & \mathrm{a}(t)^2\,r^2 & 0 \\ 0 & 0 & 0 & \mathrm{a}(t)^2\,r^2\sin(\theta)^2 \end{bmatrix},$$
$$index_char = [-1, -1]])$$

```
> tensorsGR(coords, metric, contra_metric, det_met, C1, C2, Rm, Rc,
> R, GEin, C):
> displayGR(Einstein, GEin);
```

$$\textit{The Einstein Tensor}$$
$$\textit{non} - \textit{zero components} :$$
$$G11 = -\frac{3\,((\frac{d}{dt}\,\mathrm{a}(t))^2 + k\,c^2)}{\mathrm{a}(t)^2}$$
$$G22 = -\frac{2\,\mathrm{a}(t)\,(\frac{d^2}{dt^2}\,\mathrm{a}(t)) + (\frac{d}{dt}\,\mathrm{a}(t))^2 + k\,c^2}{(-1 + k\,r^2)\,c^2}$$
$$G33 = \frac{r^2\,(2\,\mathrm{a}(t)\,(\frac{d^2}{dt^2}\,\mathrm{a}(t)) + (\frac{d}{dt}\,\mathrm{a}(t))^2 + k\,c^2)}{c^2}$$
$$G44 = \frac{r^2\sin(\theta)^2\,(2\,\mathrm{a}(t)\,(\frac{d^2}{dt^2}\,\mathrm{a}(t)) + (\frac{d}{dt}\,\mathrm{a}(t))^2 + k\,c^2)}{c^2}$$
$$character\ :\ [-1,\ -1]$$

```
> rGEin := raise(contra_metric, GEin, 1);
```

$$rGEin := \mathrm{table}([compts = \begin{bmatrix} \frac{3\,((\frac{d}{dt}\,\mathrm{a}(t))^2 + k\,c^2)}{c^2\,\mathrm{a}(t)^2} & 0 & 0 & 0 \\ 0 & \%1 & 0 & 0 \\ 0 & 0 & \%1 & 0 \\ 0 & 0 & 0 & \%1 \end{bmatrix},$$
$$index_char = [1, -1]])$$
$$\%1 := \frac{2\,\mathrm{a}(t)\,(\frac{d^2}{dt^2}\,\mathrm{a}(t)) + (\frac{d}{dt}\,\mathrm{a}(t))^2 + k\,c^2}{\mathrm{a}(t)^2\,c^2}$$

18.4.1 Evolution of the Universe

The much-discussed expansion of the universe refers to the increase in the cosmic scale factor a with respect to time t. Observationally, a is proportional to the separation between two galaxies. We can loosely consider that a is a measure of the "size of the universe." Our objective in this section is to find a as a function of t, so that we can understand the past, present and future states of the universe.

From our intuitive perspective, the universe contains stars and galaxies, but on a large scale the universe is approximately homogeneous and isotropic. To simplify the calculations, we treat the constituents of the universe as a perfect fluid. According to this approximation, we can choose a comoving frame and express the energy-momentum tensor as a diagonal matrix consisting of the energy density $\mathcal{E}$ and pressure P,

$$T^{\mu}_{\nu} = \mathrm{diag}\,(-\mathcal{E}, P, P, P)\,. \tag{18.52}$$

Because T_{00} is always positive, T^0_0 has the same sign as g^{00}, which is negative according to our definition.

The 0-0 component of the Einstein equation gives the Friedmann equation,

$$\frac{\dot{a}^2}{a^2} + \frac{kc^2}{a^2} = \frac{8\pi G}{3c^2}\mathcal{E}, \tag{18.53}$$

which governs the evolution of the universe. This first-order differential equation is in principle solvable if $\mathcal{E}$, generally a function of a, is known.

We first perform a calculation by considering a toy model: a universe consists of only matter. According to this model, the mass density $\rho = \mathcal{E}/c^2$ is inversely proportional to the volume, so $\rho = \rho_0 a^{-3}$, where ρ_0 is the mass density at present and a at present time (t_0) is set to unity. The Friedmann equation becomes

$$\frac{\dot{a}^2}{a^2} + \frac{kc^2}{a^2} = \frac{8\pi G}{3}\frac{\rho_0}{a^3}. \tag{18.54}$$

We eliminate cumbersome parameters with these substitutions: $a = [8\pi G\rho_0/(3c^2)]a_*$ and $t = [8\pi G\rho_0/(3c^3)]t_*$. With such rescaling of the coordinates, k becomes -1, 0, or $+1$ for negative, zero, or positive spatial curvature, respectively:

$$\left(\frac{da_*}{dt_*}\right)^2 + k = \frac{1}{a_*}, \quad k = -1,\ 0,\ 1. \tag{18.55}$$

This equation can be solved analytically. For $k = 0$,

$$a_* = \frac{1}{4}(12t_*)^{2/3}. \tag{18.56}$$

Worksheet 18.6 We use `dsolve` to attack the differential equation directly. Maple returns several solutions, from which we choose the real positive solution.

```
> Eq1 := diff(a(t),t)^2 = 1/a(t);
```

$$Eq1 := (\tfrac{d}{dt}\,\mathrm{a}(t))^2 = \frac{1}{\mathrm{a}(t)}$$

```
> Eq2 := dsolve({ Eq1, a(0)=0}, a(t));
```

$$Eq2 := \mathrm{a}(t) = \frac{12^{(2/3)}\,t^{(2/3)}}{4},\ \mathrm{a}(t) = \left(-\frac{12^{(1/3)}\,t^{(1/3)}}{4} + \frac{1}{4}\,I\,\sqrt{3}\,12^{(1/3)}\,t^{(1/3)}\right)^2,$$

$$\mathrm{a}(t) = \frac{(-12\,t)^{(2/3)}}{4}, \mathrm{a}(t) = \left(-\frac{(-12\,t)^{(1/3)}}{4} + \frac{1}{4}\,I\,\sqrt{3}\,(-12\,t)^{(1/3)}\right)^2,$$

$$\mathrm{a}(t) = \left(-\frac{(-12\,t)^{(1/3)}}{4} - \frac{1}{4}\,I\,\sqrt{3}\,(-12\,t)^{(1/3)}\right)^2,$$

$$\mathrm{a}(t) = \left(-\frac{12^{(1/3)}\,t^{(1/3)}}{4} - \frac{1}{4}\,I\,\sqrt{3}\,12^{(1/3)}\,t^{(1/3)}\right)^2$$

Therefore, for a flat universe dominated by matter, the size of the universe is proportional to time to the two-thirds power: $a \propto t^{2/3}$.

For $k = 1$, we also directly solve the differential equation.

Worksheet 18.7

```
> Eq1 := diff(a(t),t)^2 + 1 = 1/a(t);
```

$$Eq1 := (\tfrac{d}{dt}\,\mathrm{a}(t))^2 + 1 = \frac{1}{\mathrm{a}(t)}$$

```
> Eq2 := dsolve({Eq1, a(0)=0}, a(t));
```

$$Eq2 := \mathrm{a}(t) = -\frac{1}{2}\sin(\mathrm{RootOf}(2_Z - 4\,t + 2\,\sqrt{\cos(_Z)^2} - \pi)) + \frac{1}{2},$$

$$\mathrm{a}(t) = \frac{1}{2}\sin(\mathrm{RootOf}(-2\,_Z + 4\,t + 2\,\sqrt{\cos(_Z)^2} - \pi)) + \frac{1}{2}$$

On rearranging terms, we express this solution in parametric form. From the condition

$$-2Z + 4t_* + 2\cos Z - \pi = 0,$$

we have

$$t_* = \frac{1}{2}Z - \frac{1}{2}\cos Z + \frac{\pi}{4}.$$

Defining a parameter η as

$$\eta = Z + \frac{\pi}{2},$$

we obtain

$$t_* = \frac{1}{2}(\eta - \sin\eta), \tag{18.57a}$$

$$a_* = \frac{1}{2}(1 - \cos\eta). \tag{18.57b}$$

The solution for the case $k = -1$ can be similarly obtained with Maple. There is an alternative way to solve this problem by using η, the "conformal time," to parametrize a, which we leave as an exercise at the end of the chapter.

We summarize the solutions in three scenarios, which all have a reference point such that $a_*(t_* = 0) = 0$, of the Friedmann equation for a universe of only matter:

- flat universe ($k = 0$)

$$a_* = \frac{1}{4}(12t_*)^{2/3}; \tag{18.58}$$

- closed universe ($k > 0$)

$$t_* = \frac{1}{2}(\eta - \sin\eta), \tag{18.59a}$$

$$a_* = \frac{1}{2}(1 - \cos\eta); \tag{18.59b}$$

- open universe ($k < 0$)

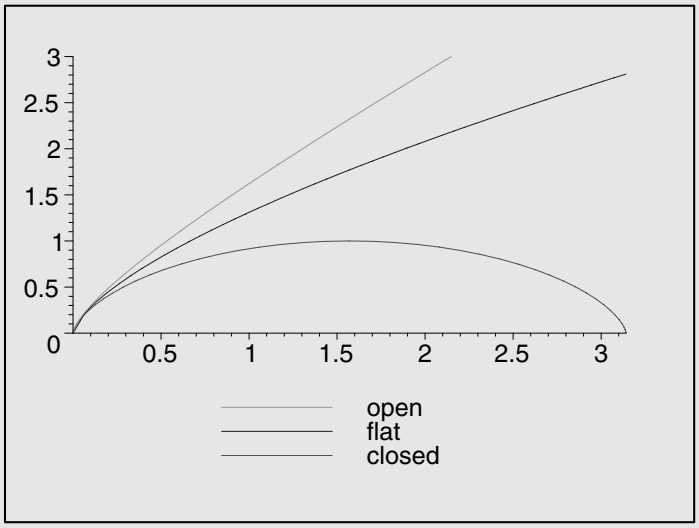
$$t_* = \frac{1}{2}(\sinh\eta - \eta), \tag{18.60a}$$

$$a_* = \frac{1}{2}(\cosh\eta - 1). \tag{18.60b}$$

We plot the dependence of the cosmic scale factor a_* on time t_* for an open, a closed and a flat universe.

Worksheet 18.8

```
> with(plots):
Warning, the name changecoords has been redefined
> p1:=plot([-1/2*(theta - sinh(theta)), -1/2*(1 - cosh(theta)),
> theta=0..2*Pi], 0..3, color=green, legend="open"):
> p2 := plot(1/4*(12*t)^(2/3), t=0..Pi, 0..3, color=blue,
> legend="flat"):
> p3 := plot([1/2*(theta - sin(theta)), 1/2*(1 - cos(theta)),
> theta=0..2*Pi], color=red, legend="closed"):
> display([p1, p2, p3]);
```



This plot demonstrates the result of general relativistic cosmology: other than at a later stage for $k > 0$, the universe is expanding. Furthermore, in all scenarios one can trace the universe back to a singularity $a = 0$, which implies infinite density and temperature; this singularity is called the *big bang*. Although currently known physical laws fail at this singularity, that fact does not preclude our defining a zero of time at this singularity merely as a reference point. According to this definition, the age of the universe is finite.

Before 1998, cosmologists thought that this toy model did indeed reflect our universe, and that the fate of the universe would depend on the intrinsic geometry: $k < 0$ for perpetual expansion, or $k > 0$ for eventual collapse. Observations of type Ia supernovae indicate that our universe is expanding at an accelerating rate![3] One implication is that the universe might

[3]A. G. Riess et al., "Observational evidence from supernovae for an accelerating universe and a cosmological

contain energy in a form similar to the cosmological constant proposed by Einstein, called the *vacuum energy*. An acceleration is understandable from the i-i component ($i = 1, 2, 3$) of the Einstein equation:

$$2\frac{\ddot{a}^2}{a} + \frac{\dot{a}^2}{a^2} + \frac{kc^2}{a^2} = -\frac{8\pi G}{c^2}P. \tag{18.61}$$

We combine this and the Friedmann equation to obtain an equation for acceleration $\ddot{a}$ only:

$$\frac{\ddot{a}^2}{a} = -\frac{4\pi G}{3c^2}(3P + \mathcal{E}). \tag{18.62}$$

The relation between $\mathcal{E}$ and P is an equation of state, for which a simple relation suffices:

$$P = w\mathcal{E}. \tag{18.63}$$

For matter, $w = 0$; for radiation, $w = 1/3$ (see Section 17.5); for vacuum energy, $w = -1$. With the vacuum energy, $3P + \mathcal{E} < 0$, thus $\ddot{a} > 0$, and expansion of the universe is accelerating. The nature of vacuum energy remains the greatest unsolved problem in physics. Any energy with $w < -1/3$, commonly refer to as the *dark energy*, causes accelerated expansion.

The first law of thermodynamics provides the relation $dU = -PdV$ for an adiabatic process. The volume is proportional to the cube of scaling factor a: $V \propto a^3$; hence we write

$$d(\mathcal{E}a^3) = -Pd(a^3) = -w\mathcal{E}d(a^3).$$

Solving this differential equation yields

$$\mathcal{E} = \rho c^2 \propto a^{-3(1+w)}. \tag{18.64}$$

To describe our universe accurately, we must consider energy in all forms: for matter, $\rho \propto a^{-3}$; for radiation, $\rho \propto a^{-4}$, and for vacuum energy, $\rho =$ constant. While the energy density contributed from matter and radiation decreases as the universe expands, that from the vacuum energy remains constant. If the vacuum energy in the above simple model ($w = -1$) is correct, it will control the destiny of our universe. A model of the universe containing only matter serves as a satisfactory approximation for much of the history of our universe, but it is inadequate to describe the future; the discussion of the connection between k and an open or closed universe discussed a few years ago was obsolete.

In observing galaxies or supernovae for cosmological investigation, astronomers measure their brightness and redshift: from the brightness of an object we deduce its distance; from the redshift we deduce the scale factor $a(t)$ at that time. A plot of redshift versus distance for a collection of supernovae constitutes a Hubble diagram, which provides a test of a solution $a(t)$ of the Friedmann equation. Astronomers prefer to express results of data reduction in terms of the Hubble parameter H_0 and dimensionless density parameter Ω_0; thus we express the Friedmann equation to conform to these quantities. The Hubble parameter is defined as

$$H \equiv \frac{\dot{a}}{a}, \tag{18.65}$$

constant," *Astronomical Journal*, **116**, 1009–1038 (1998); S. Perlmutter et al., "Measurements of Ω and Λ from 42 high-redshift supernovae," *Astrophysical Journal*, **517**, 565–586 (1999).

which is a function of time; the present value is denoted H_0. The density parameter is defined as

$$\Omega \equiv \frac{8\pi G\rho}{3H^2}, \tag{18.66}$$

which is also a function of time; with ρ_0 and H_0, its present value is Ω_0. The significance of Ω is that $\Omega = 1$ corresponds to $k = 0$, $\Omega < 1$ corresponds to $k < 0$, and $\Omega > 1$ corresponds to $k > 0$. The redshift parameter is defined as

$$1 + z = y \equiv \frac{a(t_0)}{a(t)} \equiv \frac{1}{a(t)}. \tag{18.67}$$

At present $z = 0$, so $y = 1$. It is convenient to set a to unity at the present time, t_0; i.e., $a(t_0) \equiv 1$.

According to this notation, the Friedmann equation becomes

$$H^2 + \frac{kc^2}{a^2} = H^2\Omega.$$

Because k is a constant, we express it in terms of the present values of the Hubble parameter and the density parameter,

$$kc^2 = H_0^2(\Omega_0 - 1).$$

Supposing that Ω_0 pertains to energy in the three possible forms listed above, we decompose it into

$$\Omega_0 = \Omega_\mathrm{m} + \Omega_\mathrm{r} + \Omega_\Lambda, \tag{18.68}$$

where Ω_m pertains to matter, Ω_r to radiation, and Ω_Λ to vacuum, all present values.

Each component of energy density among these three depends on the scaling factor a differently: $\rho \propto a^{-3(1+w)}$; the density ρ as a function of a is expressed as

$$\frac{8\pi G}{3}\rho = H_0^2(\Omega_\mathrm{m}a^{-3} + \Omega_\mathrm{r}a^{-4} + \Omega_\Lambda) = H_0^2(\Omega_\mathrm{m}y^3 + \Omega_\mathrm{r}y^4 + \Omega_\Lambda). \tag{18.69}$$

The Friedmann equation terms of currently observable parameters, H_0, Ω_m, Ω_r, Ω_Λ, become:

$$\boxed{\frac{\dot{a}^2}{a^2} + \frac{H_0^2(\Omega_0 - 1)}{a^2} = H_0^2(\Omega_\mathrm{m}a^{-3} + \Omega_\mathrm{r}a^{-4} + \Omega_\Lambda)}. \tag{18.70}$$

This equation includes energy in three possible forms: at an early stage when a was small, the universe was dominated by the radiation term Ω_r; as the universe expanded, it became dominated by a matter term Ω_m; it will eventually be overtaken by a vacuum energy term Ω_Λ. Although we can obtain no analytic solution of the Friedmann equation that includes energy in all possible forms, we can solve it numerically.

The solution of the Friedmann equation $a(t)$ indicates how the universe evolves; conversely, we invert the function to obtain $t(a)$, which indicates the age of the universe. To find $t_0 = t(a_0)$, we evaluate an integral:

$$t_0 = \int_0^{a(t_0)} \frac{da'}{\dot{a}'}. \tag{18.71}$$

With the following change of variables,

$$a = \frac{1}{y}, \quad da = -\frac{dy}{y^2},$$

$$\frac{1}{\dot{a}} = \frac{1}{aH} = \frac{y}{H};$$

from the Friedmann equation, we obtain

$$H = H_0[\Omega_\mathrm{m} y^3 + \Omega_\mathrm{r} y^4 + \Omega_\Lambda - (\Omega_0 - 1)y^2]^{1/2}.$$

We express equation (18.71) in terms of currently observable values:

$$\boxed{t_0 = \frac{1}{H_0} \int_1^\infty \frac{dy}{y[\Omega_\mathrm{m} y^3 + \Omega_\mathrm{r} y^4 + \Omega_\Lambda - (\Omega_0 - 1)y^2]^{1/2}}}. \tag{18.72}$$

Finally, we employ equations (18.72) and (18.70) to find the age of our universe and its evolution according to a currently popular model. As mentioned, the universe is believed to contain dark energy that accelerates its expansion. A widely used model conforming to currently available observations is a flat universe with matter and vacuum energy, ignoring the contribution of radiation ($\Omega_\mathrm{r} = 0$) because it was important for only a brief epoch in the entire history of the universe. According to this model, $\Omega_0 = 1$, or $\Omega_\Lambda + \Omega_\mathrm{m} = 1$. We have

$$t_0 = \frac{1}{H_0} \int_1^\infty \frac{dy}{y[(1 - \Omega_\Lambda)y^3 + \Omega_\Lambda]^{1/2}}. \tag{18.73}$$

We can evaluate this integral exactly:

$$t_0 = \frac{2}{3} H_0^{-1} \Omega_\Lambda^{-1/2} \ln \left[\frac{1 + \Omega_\Lambda^{1/2}}{(1 - \Omega_\Lambda)^{1/2}} \right]. \tag{18.74}$$

With a recently obtained value[4] $\Omega_\Lambda = 0.73$, and Hubble parameter $H_0 = 0.71 \times (9.77813 \text{ Gyr})^{-1}$, see Table A.2 in Appendix A, the age of the universe t_0 is 13.7 billion years.

The Friedmann equation for such a model is

$$\frac{\dot{a}^2}{a^2} = H_0^2(0.27a^{-3} + 0.73), \tag{18.75}$$

which we can solve numerically.

[4]From the Wilkinson Microwave Anisotropy Probe (*WMAP*) mission; see `http://map.gsfc.nasa.gov` and C. L. Bennett et al., *Astrophysical Journal Supplement*, **148**, 1 (2003).

Worksheet 18.9 The age of the universe, based on the model $\Omega_\Lambda + \Omega_\mathrm{m} = 1$, can be exactly integrated; the result is `Epr4`, which is measured in terms of H_0^{-1}. Adopting a commonly cited value, $H_0^{-1} = 9.77813/0.71$ Gyr. For the Friedman equation, instead of using an initial condition $a(0) = 0$ as in preceding worksheets, we shift the zero of time to the present ($t_0 = 0$) in the `dsolve` command, and use a condition $a(0) = 1$ to avoid a singularity as the initial condition for numerical solution. From the plot, we trace back to a big bang for which $a(-t_0) = 0$.

```
> assume(Omega[Lambda]>0):
> Epr1 := 1/(y*sqrt((1 - Omega[Lambda])*y^3 + Omega[Lambda]));
```

$$Epr1 := \frac{1}{y\sqrt{y^3 - y^3\,\Omega_\Lambda + \Omega_\Lambda}}$$

```
> Epr2 := int(Epr1, y=1..infinity);
```

$$Epr2 := \frac{2}{3}\,\frac{\operatorname{arcsinh}\left(\dfrac{\sqrt{\Omega_\Lambda}}{\sqrt{1-\Omega_\Lambda}}\right)}{\sqrt{\Omega_\Lambda}}$$

```
> Epr3 := convert(simplify(Epr2), ln);
```

$$Epr3 := \frac{2}{3}\,\frac{\ln\left(\dfrac{\sqrt{\Omega_\Lambda}}{\sqrt{1-\Omega_\Lambda}} + \sqrt{1 + \dfrac{\Omega_\Lambda}{1-\Omega_\Lambda}}\right)}{\sqrt{\Omega_\Lambda}}$$

```
> Epr4 := eval(Epr3, Omega[Lambda]=0.73);
```

$$Epr4 := 0.9926868740$$

```
> t0 := Epr4/0.71*9.77813;
```

$$t0 := 13.67129761$$

```
> Eq11 := diff(a(t),t) = sqrt((1 - Omega[Lambda])/a(t) +
> Omega[Lambda]*a(t)^2);
```

$$Eq11 := \tfrac{d}{dt}\,\mathrm{a}(t) = \sqrt{\frac{1-\Omega_\Lambda}{\mathrm{a}(t)} + \Omega_\Lambda\,\mathrm{a}(t)^2}$$

```
> Eq12 := eval(Eq11, Omega[Lambda]=0.73);
```

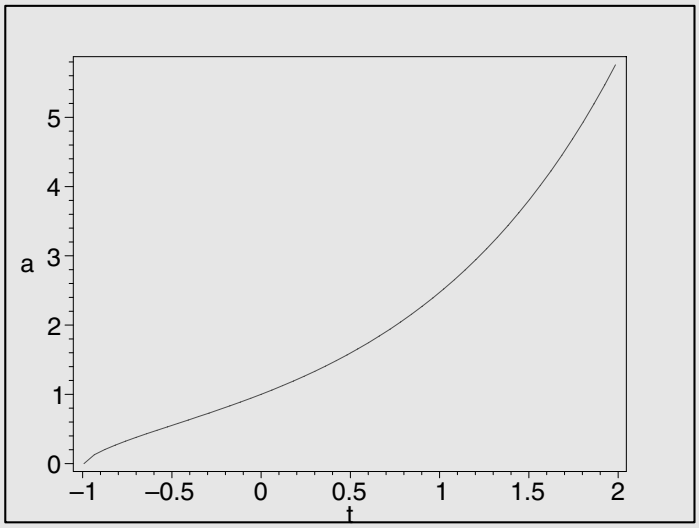
$$Eq12 := \tfrac{d}{dt}\,\mathrm{a}(t) = \sqrt{\frac{0.27}{\mathrm{a}(t)} + 0.73\,\mathrm{a}(t)^2}$$

```
> Eq13 := dsolve({Eq12, a(0)=1}, a(t), numeric);
```

$$Eq13 := \textbf{proc}(x_rkf45)\ \ldots\ \textbf{end proc}$$

```
> with(plots):
Warning, the name changecoords has been redefined
```

```
> odeplot(Eq13, [t, a(t)], -Epr4..2*Epr4, axes=BOXED);
```



If the model $\Omega_{\mathrm{m}} + \Omega_{\Lambda} = 1$ is correct, then from the plot we are currently, at time 0, in an epoch of accelerating expansion.

Exercises

1. In Section 18.1 we state that the Riemann tensor, not the Christoffel symbols, represents the intrinsic nature of geometry, and a space is flat if the Riemann tensor vanishes. Employ Maple's `tensor` package to evaluate the Christoffel symbols and components of the Riemann tensor for the metric in equation (18.5), and verify that such a space is flat but that there exist nonvanishing Christoffel symbols.

2. A centrally symmetric metric in a general form is

$$-ds^2 = -c^2 e^{\nu} dt^2 + e^{\lambda} dr^2 + r^2(d\theta^2 + \sin^2\theta d\phi^2), \tag{18.76}$$

   where both ν and λ are functions of r and t. Employ the `tensor` package to evaluate all the Christoffel symbols and components of the Einstein tensor. One can verify the answer with that in Misner et al. 1973, p. 360ff.

3. Compare the result of planetary motion in Section 18.3 based on general relativity, with that from the calculation based on Newton's law of gravitation introduced in Section 4.3.1.

4. The Kerr metric describes a rotating object; it is characterized by mass M and spin angular momentum J. In the equatorial plane, the Lagrangian is (setting $c = G = 1$)

$$L = -\frac{1}{2}\left(1 - \frac{2M}{r}\right)\dot{t}^2 - \frac{2aM}{r}\dot{t}\dot{\phi} + \frac{r^2}{2\Delta}\dot{r}^2 + \frac{1}{2}\left(r^2 + a^2 + \frac{2a^2M}{r}\right)\dot{\phi}^2, \quad (18.77)$$

where

$$a \equiv \frac{J}{M}, \quad \Delta \equiv r^2 - 2Mr + a^2. \quad (18.78)$$

Consider the motion of a particle under this metric using the technique introduced in Section 18.3.[5]

5. The Robertson–Walker metric for a space of negative curvature can alternatively be written as

$$-ds^2 = a^2(\eta)[d\eta^2 - d\chi^2 - \sinh^2\chi(d\theta^2 + \sin^2\theta\, d\phi^2)]; \quad (18.79)$$

in this form, η is the "conformal time" which is related to t as

$$d\eta = \frac{cdt}{a}. \quad (18.80)$$

(a) From this metric, verify that

$$G^0_0 = -\frac{3}{a^4}(\dot{a}^2 - a^2),$$

where the dot denotes differentiation with respect to η.

(b) The Friedman equation is thus

$$\frac{8\pi G}{c^4}\mathcal{E} = \frac{3}{a^4}(\dot{a}^2 - a^2).$$

For a matter-only universe ($\mathcal{E} \propto a^{-3}$), we rewrite the above equation as

$$C' = \frac{1}{a}(\dot{a}^2 - a^2), \quad C' \equiv \frac{8\pi G\rho a^3}{3c^2} = \text{constant}.$$

Solve this differential equation to verify that

$$a = \frac{C'}{2}(\cosh\eta - 1), \quad (18.81a)$$

and

$$t = \frac{1}{c}\int a\, d\eta = \frac{C'}{2c}(\sinh\eta - \eta). \quad (18.81b)$$

[5] See F. Y. Wang, "Relativistic orbits with computer algebra," *American Journal of Physics*, **72**, 1040–1044 (2004).

Replacing $\sinh\chi$ with $\sin\chi$ gives a space of positive curvature; repeat the above procedure and obtain equation (18.59).

6. Consider a flat universe $k = 0$ that is dominated by radiation; therefore $\mathcal{E} \propto a^{-4}$. This condition applied for the early universe; the Friedmann equation is

$$\left(\frac{da_*}{dt_*}\right)^2 = \frac{1}{a_*^2}. \tag{18.82}$$

Solve this equation to prove that $a_* \propto t^{1/2}$.

7. If the model $\Omega_{\rm m} + \Omega_\Lambda = 1$ is correct, the universe will eventually be dominated by the vacuum energy. Under these conditions, the Friedmann equation becomes

$$\left(\frac{da}{dt}\right)^2 = H_0^2 \Omega_\Lambda a^2. \tag{18.83}$$

Solve this equation to prove that $a \propto e^{\sqrt{\Omega_\Lambda} H_0 t}$.

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A Physical and Astrophysical Constants

This appendix contains values of the physical and astrophysical constants relevant to the calculations in this book; the figures in parentheses after the values give the 1-standard-deviation uncertainties in the last digits. Comprehensive tables and a discussion are available in the *Review of Particle Physics*, *Physics Letters*, **B 592**, 1 (2004), or through the internet at `http://pdg.lbl.gov`. An alternative source of physical constants recommended by the Committee on Data for Science and Technology is available at `http://physics.nist.gov/constants`.

Table A.1: Physical constants.

Quantity	**Symbol**	**Value**
speed of light in vacuum	c	$299\,792\,458$ m s^{-1}
Planck constant	h	$6.626\,068\,76(52) \times 10^{-34}$ J s
Planck constant, reduced	$\hbar \equiv h/2\pi$	$1.054\,571\,596(82) \times 10^{-34}$ J s
electron charge magnitude	e	$1.602\,176\,462(63) \times 10^{-19}$ C
electron mass	m_e	$9.109\,381\,88(72) \times 10^{-31}$ kg
proton mass	m_p	$1.672\,621\,58(13) \times 10^{-27}$ kg
unified atomic mass unit	u	$1.660\,538\,73(13) \times 10^{-27}$ kg
permeability of free space	μ_0	$4\pi \times 10^{-7}$ N A^{-2} = $12.566\ldots \times 10^{-7}$ N A^{-2}
permittivity of free space	$\epsilon_0 = 1/\mu_0 c^2$	$8.854\,187\,817\ldots \times 10^{-12}$ F m^{-1}
gravitational constant	G_N	$6.673(10) \times 10^{-11}$ m^3 kg^{-1} s^{-2}
standard gravitational acceleration	g_n	$9.806\,65$ m s^{-2}
Bohr magneton	$\mu_B = e\hbar/2m_e$	$9.274\,008\,99(37) \times 10^{-24}$ A m^2
Avogadro constant	N_A	$6.022\,141\,99(47) \times 10^{23}$ mol^{-1}
Boltzmann constant	k	$1.380\,6503(24) \times 10^{-23}$ J K^{-1}

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Table A.2: Astrophysical constants.

Quantity	**Symbol**	**Value**
solar mass	$M_\odot$	$1.9889(30) \times 10^{30}$ kg
solar equatorial radius	$R_\odot$	6.961×10^8 m
Earth mass	$M_\oplus$	$5.974(9) \times 10^{24}$ kg
Earth mean equatorial radius	$R_\oplus$	6.378140×10^6 m
parsec	pc	$3.085\,677\,5807(4) \times 10^{16}$ m
Hubble parameter†	H_0	(71^{+4}_{-3}) km s^{-1} Mpc^{-1} $= (0.71^{+0.04}_{-0.03}) \times (9.77813\ \text{Gyr})^{-1}$
cosmic background radiation temperature†	T_0	2.725 ± 0.001 K

† Subscript 0 indicates present-day values.

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B Mathematical Notes

B.1 Legendre Equation and Series Solutions

In Chapter 5, we encounter many special functions that arise as solutions of particular second-order differential equations. These solutions are obtained by expressing a trial solution as a power series. By substituting that series into the differential equation, and comparing coefficients, one deduces a recurrence relation that allows evaluation of successive coefficients.

As an illustrative example, we solve the Legendre equation first seen in Section 5.4:

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + l(l+1)y = 0. \tag{B.1.1}$$

Let the solution take the form of a power series,

$$y = \sum_{k=0}^{\infty} a_k x^k; \tag{B.1.2}$$

we directly find the first and second derivatives,

$$\frac{dy}{dx} = \sum_{k=1}^{\infty} k a_k x^{k-1}, \quad \frac{d^2y}{dx^2} = \sum_{k=2}^{\infty} k(k-1) a_k x^{k-2}. \tag{B.1.3}$$

Substituting equations (B.1.2) and (B.1.3) into the Legendre equation (B.1.1), we have

$$(1-x^2)\sum_{k=2}^{\infty} k(k-1)a_k x^{k-2} - 2x\sum_{k=1}^{\infty} k a_k x^{k-1} + l(l+1)\sum_{k=0}^{\infty} a_k x^k = 0, \tag{B.1.4}$$

and further arrangement yields

$$\sum_{k=2}^{\infty} k(k-1)a_k x^{k-2} - \sum_{k=2}^{\infty} k(k-1)a_k x^k - \sum_{k=1}^{\infty} 2k a_k x^k + l(l+1)\sum_{k=0}^{\infty} a_k x^k = 0. \tag{B.1.5}$$

For convenience in comparing coefficients, we shift the index of summation in the first term by making a change $k \to k+2$:

$$\sum_{k=0}^{\infty} (k+2)(k+1)a_{k+2} x^k - \sum_{k=2}^{\infty} k(k-1)a_k x^k - \sum_{k=1}^{\infty} 2k a_k x^k + l(l+1)\sum_{k=0}^{\infty} a_k x^k = 0. \tag{B.1.6}$$

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Collecting coefficients of the term x^k, we discover that, for any $k \geq 2$, the condition

$$a_{k+2} = \frac{k(k-1) + 2k - l(l+1)}{(k+2)(k+1)} a_k \tag{B.1.7}$$

must be satisfied. This formula is the recurrence relation, according to which we can evaluate successive coefficients.

Deriving the recurrence relation involves a straightforward, but typically tedious, comparison of coefficients. For a second-order differential equation, one can employ Maple to generate a sum containing five consecutive terms, then collect coefficients to produce the recurrence relation.

Worksheet B.1 We write a polynomial that is a sum of five terms, and insert this directly into the differential equation. With Maple's command `coeff` we collect coefficients of x to kth power to derive the recurrence relation.

```
> y := sum(a[i]*x^i, i=k-2..k+2);
```

$$y := a_{k-2}\, x^{(k-2)} + a_{-1+k}\, x^{(-1+k)} + a_k\, x^k + a_{1+k}\, x^{(1+k)} + a_{k+2}\, x^{(k+2)}$$

```
> EqP := (1-x^2)*diff(y,x$2) - 2*x*diff(y,x) + l*(l+1)*y=0:
> Eq1 := simplify(EqP):
> Eq2 := map(coeff, Eq1, x^k);
```

$$Eq2 := 2\, a_{k+2} + a_{k+2}\, k^2 + 3\, a_{k+2}\, k + l\, a_k + l^2\, a_k - a_k\, k^2 - a_k\, k = 0$$

```
> Eq3 := isolate(Eq2, a[k+2]);
```

$$Eq3 := a_{k+2} = \frac{-l\, a_k - l^2\, a_k + a_k\, k^2 + a_k\, k}{2 + k^2 + 3\, k}$$

```
> Eq4 := factor(Eq3);
```

$$Eq4 := a_{k+2} = -\frac{a_k\, (l + 1 + k)\, (l - k)}{(k + 2)\, (1 + k)}$$

Maple rearranges the recurrence relation to give

$$a_{k+2} = \frac{(k+l+1)(k-l)}{(k+2)(k+1)} a_k. \tag{B.1.7$'$}$$

Although our solution is originally expressed as an infinite series, if l is a positive integer, the series terminates when $k = l$. Therefore, an infinite series as a solution to the Legendre equation becomes a polynomial of degree l if l is zero or a positive integer.

We must exercise care about the lowest terms, i.e., the constant term and the linear term, because they might not conform to the recurrence relation. For this problem, the constant term, with $k = 0$, gives

$$a_2 = -\frac{l(l+1)}{2} a_0, \tag{B.1.8}$$

and the next term, with $k = 1$, gives

$$a_3 = \frac{2 - l(l+1)}{6} a_1; \tag{B.1.9}$$

both terms conform to a general recurrence relation. Because the recurrence relation relates a_{k+2} and a_k (second one before), we have an even series with coefficients a_0, a_2, a_4, ..., and an odd series with coefficients a_1, a_3, a_5, ... We employ Maple to find explicit solutions for the Legendre equation when l is a positive integer.

Worksheet B.2 We define a polynomial explicitly, and insert it into the Legendre equation, from which we find the recurrence relation. For the even series, we set $a_0 = 1$ and $a_1 = 0$; for the odd series we set $a_0 = 0$ and $a_1 = 1$. For a positive integer l, we obtain solutions expressed as a polynomial of degree l. A simple `FOR` loop serves to generate the polynomials.

```
> y := add(a[i]*x^i, i=0..8);
```

$$y := a_0 + a_1\,x + a_2\,x^2 + a_3\,x^3 + a_4\,x^4 + a_5\,x^5 + a_6\,x^6 + a_7\,x^7 + a_8\,x^8$$

```
> Eq11 := (1-x^2)*diff(y,x$2) - 2*x*diff(y,x) + l*(l+1)*y=0;
```

$$\begin{aligned} Eq11 :=\ & (1-x^2)\,(2\,a_2 + 6\,a_3\,x + 12\,a_4\,x^2 + 20\,a_5\,x^3 + 30\,a_6\,x^4 + 42\,a_7\,x^5 + 56\,a_8\,x^6) \\ & - 2\,x\,(a_1 + 2\,a_2\,x + 3\,a_3\,x^2 + 4\,a_4\,x^3 + 5\,a_5\,x^4 + 6\,a_6\,x^5 + 7\,a_7\,x^6 + 8\,a_8\,x^7) \\ & + l\,(l+1)\,(a_0 + a_1\,x + a_2\,x^2 + a_3\,x^3 + a_4\,x^4 + a_5\,x^5 + a_6\,x^6 + a_7\,x^7 + a_8\,x^8) = 0 \end{aligned}$$

```
> Eq12 := collect(Eq11, x);
```

$$\begin{aligned} Eq12 :=\ & (-72\,a_8 + l\,(l+1)\,a_8)\,x^8 + (-56\,a_7 + l\,(l+1)\,a_7)\,x^7 \\ & + (56\,a_8 - 42\,a_6 + l\,(l+1)\,a_6)\,x^6 + (-30\,a_5 + 42\,a_7 + l\,(l+1)\,a_5)\,x^5 \\ & + (l\,(l+1)\,a_4 - 20\,a_4 + 30\,a_6)\,x^4 + (-12\,a_3 + 20\,a_5 + l\,(l+1)\,a_3)\,x^3 \\ & + (12\,a_4 - 6\,a_2 + l\,(l+1)\,a_2)\,x^2 + (6\,a_3 + l\,(l+1)\,a_1 - 2\,a_1)\,x + 2\,a_2 + l\,(l+1)\,a_0 \\ = & 0 \end{aligned}$$

```
> a[2] := -l*(l+1)/2*a[0];
```

$$a_2 := -\frac{1}{2}\,l\,(l+1)\,a_0$$

```
> for i from 1 to 6 do
> map(coeff, Eq12, x^i);
> isolate(%, a[i+2]);
> assign(%);
> end do:
> a[1] := 0; a[0] := 1;
```

$$a_1 := 0$$
$$a_0 := 1$$

```
> for l from 0 by 2 to 8 do y end do;
```

$$1$$

$$1 - 3\,x^2$$

$$1 - 10\,x^2 + \frac{35}{3}\,x^4$$

$$1 - 21\,x^2 + 63\,x^4 - \frac{231}{5}\,x^6$$

$$1 - 36\,x^2 + 198\,x^4 - \frac{1716}{5}\,x^6 + \frac{1287}{7}\,x^8$$

```
> a[0] := 0; a[1] := 1;
```

$$a_0 := 0$$

$$a_1 := 1$$

```
> for l from 1 by 2 to 7 do y end do;
```

$$x$$

$$x - \frac{5}{3}\,x^3$$

$$x - \frac{14}{3}\,x^3 + \frac{21}{5}\,x^5$$

$$x - 9\,x^3 + \frac{99}{5}\,x^5 - \frac{429}{35}\,x^7$$

In Table B.1 we list several solutions that are called Legendre polynomials $P_l(x)$. Note that our listing here differs from Table 5.1 by a constant factor.

Table B.1: Solutions to the Legendre equation.

l	Solution
0	1
1	x
2	$1 - 3x^2$
3	$x - \frac{5}{3}x^3$
4	$1 - 10x^2 + \frac{35}{3}x^4$
5	$x - \frac{14}{3}x^3 + \frac{21}{5}x^5$

B.2 Whittaker Function and Hypergeometric Series

If we use Maple to directly solve those well-known Schrödinger equations that admit analytic solutions, we often obtain the Whittaker function. In this section we first discuss the Whittaker functions and their connection to the hypergeometric series, then apply this knowledge to three common problems in quantum mechanics.

The Whittaker equation is

$$\frac{d^2W(x)}{dx^2} + \left(-\frac{1}{4} + \frac{k}{x} + \frac{\frac{1}{4} - m^2}{x^2}\right) W(x) = 0; \tag{B.2.1}$$

its solution is

$$M_{k,m}(x) = x^{1/2+m} e^{-x/2} \left[1 + \frac{\frac{1}{2} + m - k}{1!(2m+1)} x + \frac{(\frac{1}{2} + m - k)(\frac{3}{2} + m - k)}{2!(2m+1)(2m+2)} x^2 + \ldots\right]. \tag{B.2.2}$$

This solution can be written in terms of the confluent hypergeometric function, defined as

$$F(\alpha, \gamma; x) = 1 + \frac{\alpha}{\gamma}\frac{x}{1!} + \frac{\alpha(\alpha+1)}{\gamma(\gamma+1)}\frac{x^2}{2!} + \ldots. \tag{B.2.3}$$

The solution $M_{k,m}(x)$ thus becomes

$$M_{k,m}(x) = e^{-x/2} x^{m+1/2} F\left(\frac{1}{2} + m - k, 1 + 2m; x\right). \tag{B.2.4}$$

In the preceding section we have learned that we can solve a differential equation using power series; therefore it is not surprising that a solution to the Whittaker equation can be expressed as a hypergeometric function, which is a power series.

We employ Maple to solve the Whittaker equation directly.

Worksheet B.3

```
> Eq1 := diff(W(x), x$2) + (-1/4 + k/x + (1/4 - m^2)/x^2)*W(x) = 0;
```

$$Eq1 := \left(\tfrac{d^2}{dx^2}\,\mathrm{W}(x)\right) + \left(-\frac{1}{4} + \frac{k}{x} + \frac{\frac{1}{4} - m^2}{x^2}\right)\mathrm{W}(x) = 0$$

```
> Soln1 := dsolve(Eq1, W(x));
```

$$Soln1 := \mathrm{W}(x) = _C1\ \mathrm{WhittakerM}(k,\ m,\ x) + _C2\ \mathrm{WhittakerW}(k,\ m,\ x)$$

Because the Whittaker equation is a second-order differential equation, there must exist a second independent solution. From the symmetry of m, which appears as m^2 in the differential equation, another solution is readily obtained as $M_{k,-m}(x)$. Maple returns two functions:

`WhittakerM` and `WhittakerW`. From Maple's help facility, one finds that `WhittakerM` can be converted to a hypergeometric function as stated above. The second solution `WhittakerW` is related to `KummerU`, which is not explicitly defined in Maple help. Instead of using $M_{k,-m}(x)$ as the second solution, `WhittakerW` is actually a combination of $M_{k,m}(x)$ and $M_{k,-m}(x)$:

$$W_{k,m}(x) = \frac{\Gamma(-2m)}{\Gamma(\frac{1}{2} - m - k)} M_{k,m}(x) + \frac{\Gamma(2m)}{\Gamma(\frac{1}{2} + m - k)} M_{k,-m}(x). \tag{B.2.5}$$

Although not directly affecting our discussion of quantum mechanics, we consider a somewhat complicated situation of the Whittaker equation. Using the power series to find solutions, we must remain aware of the singular point. Near a singular point, instead of writing a general solution such as equation (B.1.2), we must use

$$y = x^q \sum_{k=0}^{\infty} a_k x^k, \tag{B.2.6}$$

where q is to be determined by the indicial equation; see our discussion of the Coulomb potential in Section 16.4. There is a mathematical theorem that, if roots (say r_1 and r_2) of the indicial equation differ by an integer, the solutions in the form of equation (B.2.6) are not independent of each other. In the current example, if $2m$ is an integer, then $M_{k,m}(x)$ and $M_{k,-m}(x)$ are not independent. To find the second independent solution, one needs to include a logarithmic term:[1]

$$y_2 = g y_1 \ln|x| + |x|^{r_2} \left[1 + \sum_{k=1}^{\infty} c_k x^k \right], \tag{B.2.7a}$$

where

$$y_1 = |x|^{r_1} \sum_{k=0}^{\infty} a_k x^k. \tag{B.2.7b}$$

The coefficients g, a_k and c_k can be determined by the method introduced in the preceding section. We refrain from elaborating this equation further, because for most physical applications the second solution is unsuitable. The situation is similar to the Bessel functions, for which we typically use the Bessel function of the first kind $J_\nu(x)$, not of the second kind $Y_\nu(x)$ because the latter diverges at the origin.

B.2.1 Harmonic Oscillator

We use Maple to solve the problem of the harmonic oscillator; the pertinent differential equation is

$$-\frac{\hbar^2}{2\mu} \frac{d^2\psi(x)}{dx^2} + \frac{1}{2}\mu\omega^2 x^2 \psi(x) = E\psi(x). \tag{B.2.8}$$

[1] Boyce and Diprima 2001, p. 277ff.

Worksheet B.4

```
> Eq1 := -h_^2/(2*mu)*diff(psi(x), x$2) + 1/2*mu*omega^2*x^2*psi(x)
> = En*psi(x);
```

$$Eq1 := -\frac{1}{2}\frac{h_^2\left(\frac{d^2}{dx^2}\psi(x)\right)}{\mu} + \frac{1}{2}\mu\,\omega^2\,x^2\,\psi(x) = En\,\psi(x)$$

```
> Soln1 := dsolve(Eq1, psi(x));
```

$$Soln1 := \psi(x) = \frac{_C1\ \text{WhittakerM}\left(\frac{En}{2\,\omega\,h_},\ \frac{1}{4},\ \frac{\mu\,\omega\,x^2}{h_}\right)}{\sqrt{x}} + \frac{_C2\ \text{WhittakerW}\left(\frac{En}{2\,\omega\,h_},\ \frac{1}{4},\ \frac{\mu\,\omega\,x^2}{h_}\right)}{\sqrt{x}}$$

According to this Maple output, we obtain functions `WhittakerM` and `WhittakerW`; we retain the former. First, we define a parameter ξ,

$$\xi = \sqrt{\frac{\mu\omega}{\hbar}}x, \tag{B.2.9}$$

then convert `WhittakerM` into a hypergeometric function. With this notation,

$$M_{k,m}(z) \equiv M(k;m;z), \tag{B.2.10}$$

from Maple we have

$$\frac{1}{\sqrt{\xi}}M\left(\frac{1}{2}\frac{E}{\hbar\omega};\frac{1}{4};\xi^2\right) = \frac{1}{\sqrt{\xi}}e^{-\xi/2}\xi^{3/2}F\left(\frac{3}{4}-\frac{1}{2}\frac{E}{\hbar\omega},\frac{3}{2};\xi^2\right), \tag{B.2.11}$$

and the other solution is

$$\frac{1}{\sqrt{\xi}}M\left(\frac{1}{2}\frac{E}{\hbar\omega};-\frac{1}{4};\xi^2\right) = \frac{1}{\sqrt{\xi}}e^{-\xi/2}\xi^{1/2}F\left(\frac{1}{4}-\frac{1}{2}\frac{E}{\hbar\omega},\frac{1}{2};\xi^2\right). \tag{B.2.12}$$

Examining the hypergeometric functions, we see that, if α is a negative integer or zero, $F(\alpha,\gamma,z)$ reduces to a polynomial of degree $|\alpha|$. We have encountered this condition in attacking the Hermite equation in Section 15.4, for which the series terminates only if λ is zero or a positive integer. From the first solution, we must have

$$\frac{3}{4}-\frac{1}{2}\frac{E}{\hbar\omega} = -n, \quad E_n = \left[(2n+1)+\frac{1}{2}\right]\hbar\omega, \tag{B.2.13}$$

and from the second solution, we must have

$$\frac{1}{4}-\frac{1}{2}\frac{E}{\hbar\omega} = -n, \quad E_n = \left(2n+\frac{1}{2}\right)\hbar\omega, \tag{B.2.14}$$

where n is an integer, so that the solution remains finite when x approaches infinity. Combining these formulas, we obtain discrete energies as

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{B.2.15}$$

We can express the Hermite polynomials in terms of the hypergeometric functions, namely

$$H_{2n}(z) = (-1)^n \frac{(2n)!}{n!} F\left(-n, \frac{1}{2}; z^2\right), \tag{B.2.16}$$

and

$$H_{2n+1}(z) = (-1)^n \frac{(2n+1)!}{n!} 2z F\left(-n, \frac{3}{2}; z^2\right). \tag{B.2.17}$$

We thus have the wave functions of the harmonic oscillator. According to this example, we conclude that careful analysis of the Maple output enables us to obtain solutions of the Schrödinger equation in certain cases.

B.2.2 Morse Potential

We apply the `dsolve` command to solve the Schrödinger equation for the Morse oscillator:

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi(x)}{dx^2} + V_0(1 - e^{-\alpha x})^2\psi(x) = E\psi(x). \tag{B.2.18}$$

Worksheet B.5

```
> Eq1 := -h_^2/(2*mu)*diff(psi(x), x$2)
> + V0*(1 - exp(-alpha*x))^2*psi(x) = En*psi(x);
```

$$Eq1 := -\frac{1}{2}\frac{h_^2\left(\frac{d^2}{dx^2}\psi(x)\right)}{\mu} + V0\,(1 - e^{(-\alpha\,x)})^2\,\psi(x) = En\,\psi(x)$$

```
> Soln1 := dsolve(Eq1, psi(x));
```

$$Soln1 := \psi(x) =$$

$$_C1\, e^{\left(\frac{\alpha\,x}{2}\right)}\,\mathrm{WhittakerM}\left(\frac{\sqrt{2}\,\sqrt{\mu}\,\sqrt{V0}}{\alpha\,h_}, \frac{\sqrt{2}\,\sqrt{\mu}\,\sqrt{V0 - En}}{\alpha\,h_}, \frac{2\,\sqrt{2}\,\sqrt{\mu}\,\sqrt{V0}\,e^{(-\alpha\,x)}}{\alpha\,h_}\right)$$

$$+_C2\, e^{\left(\frac{\alpha\,x}{2}\right)}\,\mathrm{WhittakerW}\left(\frac{\sqrt{2}\,\sqrt{\mu}\,\sqrt{V0}}{\alpha\,h_}, \frac{\sqrt{2}\,\sqrt{\mu}\,\sqrt{V0 - En}}{\alpha\,h_}, \frac{2\,\sqrt{2}\,\sqrt{\mu}\,\sqrt{V0}\,e^{(-\alpha\,x)}}{\alpha\,h_}\right)$$

We again obtain `WhittakerM` and `WhittakerW`, of which we discuss the former. Defining

$$\xi = \frac{2\sqrt{2\mu V_0}}{\alpha\hbar}e^{-\alpha x}, \quad s = \frac{\sqrt{2\mu(V_0 - E)}}{\alpha\hbar}, \tag{B.2.19}$$

we convert `WhittakerM` to a hypergeometric function,

$$\begin{aligned}&\frac{1}{\sqrt{\xi}}M\left(\frac{\sqrt{2\mu V_0}}{\alpha\hbar}; \frac{\sqrt{2\mu(V_0 - E)}}{\alpha\hbar}; \xi\right) \\ &= \frac{1}{\sqrt{\xi}}e^{-\xi/2}\xi^{s+1/2}F\left(\frac{1}{2} + \frac{\sqrt{2\mu(V_0 - E)}}{\alpha\hbar} - \frac{\sqrt{2\mu V_0}}{\alpha\hbar}, 1 + 2\frac{\sqrt{2\mu(V_0 - E)}}{\alpha\hbar}; \xi\right).\end{aligned} \tag{B.2.20}$$

To have the hypergeometric function terminate at one term, we must have

$$\frac{1}{2} + \frac{\sqrt{2\mu(V_0 - E)}}{\alpha\hbar} - \frac{\sqrt{2\mu V_0}}{\alpha\hbar} = -n, \tag{B.2.21}$$

where n is an integer. From this result, we obtain the discrete energies,

$$E_n = \hbar\sqrt{\frac{2V_0\alpha^2}{\mu}}\left(n + \frac{1}{2}\right) - \frac{\alpha^2\hbar^2}{2\mu}\left(n + \frac{1}{2}\right)^2. \tag{B.2.22}$$

Adopting the abbreviated notation above, we express the wave function as

$$\psi_n(x) = e^{-\xi/2}\xi^s F(-n, 2s + 1; \xi). \tag{B.2.23}$$

In Section 15.7, we plot these wave functions.

B.2.3 Coulomb Potential

The radial equation that arises in a wave-mechanical treatment of the hydrogen atom is

$$-\frac{\hbar^2}{2\mu r^2}\frac{d}{dr}\left[r^2\frac{dR(r)}{dr}\right] + \left[\frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r}\right]R(r) = ER(r). \tag{B.2.24}$$

Worksheet B.6

```
> Eq1 := -h^2/(8*Pi^2*mu*r^2)*diff(r^2*diff(R(r), r), r)
> + (l*(l+1)*h^2/(8*Pi^2*mu*r^2) - e^2/(4*Pi*epsilon*r))*R(r)
> = -En*R(r);
```

$$\begin{aligned}Eq1 := &-\frac{1}{8}\frac{h^2\left(2\,r\left(\frac{d}{dr}\mathrm{R}(r)\right) + r^2\left(\frac{d^2}{dr^2}\mathrm{R}(r)\right)\right)}{\pi^2\,\mu\,r^2} + \left(\frac{l\,(l+1)\,h^2}{8\,\pi^2\,\mu\,r^2} - \frac{e^2}{4\,\pi\,\varepsilon\,r}\right)\mathrm{R}(r) \\ &= -En\,\mathrm{R}(r)\end{aligned}$$

```
> Soln1 := dsolve(Eq1, R(r));
```

$$Soln1 := \mathrm{R}(r) = \frac{_C1\ \mathrm{WhittakerM}\left(\frac{e^2\sqrt{\mu}\sqrt{2}}{4\,h\,\varepsilon\sqrt{En}},\ l+\frac{1}{2},\ \frac{4\sqrt{2}\,\pi\sqrt{En}\sqrt{\mu}\,r}{h}\right)}{r} + \frac{_C2\ \mathrm{WhittakerW}\left(\frac{e^2\sqrt{\mu}\sqrt{2}}{4\,h\,\varepsilon\sqrt{En}},\ l+\frac{1}{2},\ \frac{4\sqrt{2}\,\pi\sqrt{En}\sqrt{\mu}\,r}{h}\right)}{r}$$

Maple again provides two solutions, `WhittakerM` and `WhittakerW`, and only the former is relevant in our discussion. Defining

$$\rho = \frac{2\pi\sqrt{2\mu E}}{h} r, \tag{B.2.25}$$

we convert the solution to a hypergeometric function as

$$\frac{1}{\rho} M\left(-\frac{\sqrt{2\mu}e^2}{4h\epsilon_0\sqrt{E}}; l+\frac{1}{2}; 2\rho\right) = e^{-\rho}\rho^l F\left(l+1+\frac{\sqrt{2\mu}e^2}{4h\epsilon_0\sqrt{E}}, 2l+2; 2\rho\right). \tag{B.2.26}$$

To ensure that the series terminates at one term, we must have

$$l+1+\frac{\sqrt{2\mu}e^2}{4h\epsilon_0\sqrt{E}} = -n_r, \tag{B.2.27}$$

where n_r is an integer. Let $n = n_r + l + 1$; the discrete energies become

$$E_n = -\frac{1}{n^2}\frac{\mu e^4}{8h^2\epsilon_0^2}. \tag{B.2.28}$$

This result, the same as from Bohr's model, is expected. We let the reader verify that Laguerre polynomials can be converted to a hypergeometric series,

$$L_{n+l}^{2l+1}(\rho) = \frac{[(n+l)!]^2}{(n-l-1)!(2l+1)!} F(l+1-n, 2l+2; \rho). \tag{B.2.29}$$

We express the radial part of the wave function for the hydrogen atom in terms of Laguerre polynomials in Section 16.5.

Exercise Prove that for the potential

$$V(x) = \mathcal{A}\left(\frac{a}{x} - \frac{x}{a}\right)^2, \quad \text{for } x > 0, \tag{B.2.30}$$

the energy levels are

$$E_n = \hbar\sqrt{\frac{8\mathcal{A}}{ma^2}}\left[\left(n+\frac{1}{2}\right) + \frac{1}{4}\left(\sqrt{1+\frac{8m\mathcal{A}a^2}{\hbar^2}} - \sqrt{\frac{8m\mathcal{A}a^2}{\hbar^2}}\right)\right]. \tag{B.2.31}$$

For this potential, sometimes referred to as the Davidson–Klein potential, intervals between adjacent energy levels are equal, like those of the harmonic oscillator, but with a greater residual energy.

B.3 Clausius–Mossotti Equation

We derive the Clausius–Mossotti equation mentioned in Section 13.5, which relates the dielectric constant to the atomic polarizability. As definitions of dielectric quantities are not universally agreed, and as units in various systems might cause confusion, we first clarify the terminology. Adopting SI units, the electric displacement $\mathbf{D}$ is defined as

$$\mathbf{D} \equiv \epsilon_0 \mathbf{E} + \mathbf{P}. \tag{B.3.1}$$

In linear media, the polarization $\mathbf{P}$ is proportional to the electric field $\mathbf{E}$:

$$\mathbf{P} = \epsilon_0 \chi_e \mathbf{E}, \tag{B.3.2}$$

where ϵ_0 is the permittivity of free space and χ_e is the electric susceptibility. When this equation holds, typically when the field is weak, the electric displacement becomes proportional to the electric field,

$$\mathbf{D} = \epsilon \mathbf{E}, \tag{B.3.3}$$

where ϵ is the permittivity; we must be aware that this equation is valid for a linear medium only. We further define the dielectric constant, or relative permittivity, for such a linear medium,

$$\epsilon_r \equiv \frac{\epsilon}{\epsilon_0} = 1 + \chi_e = 1 + \frac{\mathbf{P}}{\epsilon_0 \mathbf{E}}; \tag{B.3.4}$$

which is the ratio of the permittivity to the permittivity of free space.

When an atom is placed in an electric field, a dipole moment $\mathbf{p}$ is induced. The atomic polarizability is defined as

$$\mathbf{p} = \alpha \mathbf{E}_{\text{local}}. \tag{B.3.5}$$

The polarization $\mathbf{P}$ signifies the total net dipole moment per unit volume; with n atoms per unit volume, we have

$$\mathbf{P} = n\mathbf{p} = n\alpha \mathbf{E}_{\text{local}}. \tag{B.3.6}$$

The origin of an induced dipole is that an atomic nucleus is displaced in the direction of the field, while the electronic density is displaced in the opposite way. For this reason, we denote $\mathbf{E}_{\text{local}}$ for the field experienced by a particular atom, which differs from the averaged macroscopic field $\mathbf{E}$.

Determination of a local field $\mathbf{E}_{\text{local}}$ is complicated because it combines the effects of the externally applied field and the fields produced by neighboring atoms. For a gaseous sample at low density, we can ignore the latter because atoms are far apart from each other, and use the macroscopic field $\mathbf{E}$ as local field $\mathbf{E}_{\text{local}}$. The dielectric constant is related to the polarizability as

$$P = n\alpha E, \quad \chi_e = \epsilon_r - 1 = \frac{P}{\epsilon_0 E} = \frac{n\alpha}{\epsilon_0}. \tag{B.3.7}$$

For a condensed state, interactions between atoms play an important role. We express the local field as

$$\mathbf{E}_{\text{local}} = \mathbf{E} + \mathbf{E}_1, \tag{B.3.8}$$

where $\mathbf{E}_1$ accounts for contributions from neighboring atoms. According to a simplified model, a polarized medium under uniform field $\mathbf{E}$ develops uniform $\mathbf{P}$, and each atom occupies a spherical cavity. To calculate the electric field inside a spherical cavity, we need to consider merely the surface charge density on the sphere, which is the "bound charge" discussed in most textbooks on electromagnetism.[2] Choosing the z axis to coincide with the direction of $\mathbf{P}$, we express the surface charge density as

$$\sigma_b = \mathbf{P} \cdot \hat{\mathbf{n}} = P \cos\theta. \tag{B.3.9}$$

Recall Coulomb's law in equation (6.7):

$$\mathbf{E}(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0} \int \frac{\sigma(\mathbf{r}_2)}{r_{12}^2} \, \mathbf{e}_{12} \, da_2. \tag{B.3.10}$$

With σ_b for $\sigma(\mathbf{r}_2)$, at the center of the spherical cavity, r_{12} is the radius R; the z component of the unit vector $\mathbf{e}_{12}$ is $\cos\theta$; the area element is $da_2 = 2\pi R^2 \sin\theta \, d\theta$. We evaluate the electric field to be

$$E_z = \frac{1}{4\pi\epsilon_0} \int_0^\pi \frac{P\cos\theta}{R^2} \cos\theta (2\pi R^2 \sin\theta) \, d\theta = \frac{P}{3\epsilon_0}. \tag{B.3.11}$$

We conclude that the field in a spherical cavity is greater than the average field by an amount $P/3\epsilon_0$.

To proceed to relate atomic polarizability to dielectric constant, the local field according to the above approximation is

$$E_{\text{local}} = E + E_1 = E + \frac{1}{3\epsilon_0} P; \tag{B.3.12}$$

therefore equation (B.3.6) becomes

$$P = n\alpha E_{\text{local}} = n\alpha \left(E + \frac{1}{3\epsilon_0} P \right). \tag{B.3.13}$$

[2] Griffiths 1999, p. 167.

With the dielectric constant as defined in equation (B.3.4):

$$\epsilon_r = 1 + \frac{P}{\epsilon_0 E}. \tag{B.3.14}$$

we obtain the Clausius–Mossotti relation:

$$\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{n}{3\epsilon_0}\alpha. \tag{B.3.15}$$

Worksheet B.7 The calculations in this worksheet are straightforward.

```
> E1 :=
> 1/(4*Pi*epsilon[0])*int(P*cos(theta)/R^2*cos(theta)*2*Pi*R^2
> *sin(theta), theta=0..Pi);
```

$$E1 := \frac{1}{3}\frac{P}{\varepsilon_0}$$

```
> E[loc] := E + E1;
```

$$E_{loc} := E + \frac{1}{3}\frac{P}{\varepsilon_0}$$

```
> Eq1 := P = n*alpha*E[loc];
```

$$Eq1 := P = n\,\alpha\left(E + \frac{1}{3}\frac{P}{\varepsilon_0}\right)$$

```
> Eq2 := epsilon[r] = 1 + P/(epsilon[0]*E);
```

$$Eq2 := \varepsilon_r = 1 + \frac{P}{\varepsilon_0 E}$$

```
> Eq3 := solve({Eq1, Eq2}, {alpha, P});
```

$$Eq3 := \left\{P = \varepsilon_r\,\varepsilon_0\,E - \varepsilon_0\,E,\ \alpha = \frac{3\,\varepsilon_0\,(\varepsilon_r - 1)}{n\,(2 + \varepsilon_r)}\right\}$$

The Clausius–Mossotti equation works reasonably well for gases and liquids consisting of non polar molecules. To apply it solids, one must consider crystalline structure; see reference.[3] Modifying the Clausius–Mossotti equation to take into account a contribution of molecules with permanent dipole moments produces the Debye equation for dielectric constant; see Section 13.5. The shortcomings of the Clausius–Mossotti relation root from the oversimplified assumption about the local field; a correct expression for this local field is a vexing issue, which is a topic of condensed matter physics.

In Section 10.6, we state that the speed of light in a vacuum is

$$c = \frac{1}{\sqrt{\mu_0\epsilon_0}}; \tag{B.3.16}$$

[3] C. Kittel, *Introduction to Solid State Physics*, 7th ed., New York: Wiley, 1996, p. 390.

the speed of light in media is naturally

$$v = \frac{1}{\sqrt{\mu\epsilon}}. \tag{B.3.17}$$

In optics, the index of refraction is defined as

$$n_o = \frac{c}{v}; \tag{B.3.18}$$

thus the index of refraction is the square root of the dielectric constant:

$$n_o = \frac{\sqrt{\mu\epsilon}}{\sqrt{\mu_0\epsilon_0}} = \sqrt{\epsilon_r}, \quad (\mu = \mu_0). \tag{B.3.19}$$

To relate the index of refraction to the atomic polarizability, equation (B.3.7) becomes

$$n_0 = \sqrt{1 + \frac{n\alpha}{\epsilon_0}} \cong 1 + \frac{n\alpha}{2\epsilon_0}, \tag{B.3.20}$$

which is applicable to nonpolar molecules in a dilute gaseous state. We obtain the Lorenz–Lorentz equation directly from the Clausius–Mossotti equation,

$$\frac{n_o^2 - 1}{n_o^2 + 2} = \frac{n}{3\epsilon_0}\alpha, \tag{B.3.21}$$

which applies to nonpolar molecules in a condensed state.

B.4 Bose–Einstein Integral Function

This section closely follows a method demonstrated by Robinson.[4]

The Bose–Einstein integral function is defined as

$$g_\sigma(z) = \frac{1}{\Gamma(\sigma)} \int_0^\infty \frac{x^{\sigma-1}}{e^x z^{-1} - 1}\, dx. \tag{B.4.1}$$

We expand this integral as a series in z to the positive powers,

$$g_\sigma(z) = z + \frac{z^2}{2^\sigma} + \frac{z^3}{3^\sigma} + \frac{z^4}{4^\sigma} + \ldots. \tag{B.4.2}$$

When $z \cong 1$, it is more suitable to use another parameter

$$\alpha = -\ln z, \tag{B.4.3}$$

[4] J. E. Robinson, "Note on the Bose–Einstein integral functions," *Physical Review*, **83**, 678–679 (1951).

which is a small positive number. The series becomes

$$g_\sigma(\alpha) = e^{-\alpha} + \frac{e^{-2\alpha}}{2^\sigma} + \frac{e^{-3\alpha}}{3^\sigma} + \frac{e^{-4\alpha}}{4^\sigma} + \dots . \tag{B.4.4}$$

Applying the Mellin transformation to $g_\sigma(\alpha)$, defined as

$$\mathcal{G}(\sigma, s) = \int_0^\infty g_\sigma(\alpha)\alpha^{s-1}d\alpha = \int_0^\infty \sum_{m=1}^{\infty} \frac{e^{-m\alpha}}{m^\sigma}\alpha^{s-1}d\alpha, \tag{B.4.5}$$

we can evaluate each term of the integral,

$$\mathcal{G}(\sigma, s) = \Gamma(s) + \frac{\Gamma(s)}{2^{s+\sigma}} + \frac{\Gamma(s)}{3^{s+\sigma}} + \frac{\Gamma(s)}{4^{s+\sigma}} + \dots ;$$

from this trend, we deduce that the series is a product of a gamma function and a Riemann zeta function,

$$\mathcal{G}(\sigma, s) = \Gamma(s)\zeta(s + \sigma). \tag{B.4.6}$$

The inverse Mellin transformation is defined as

$$g_\sigma(\alpha) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \mathcal{G}(\sigma, s)\alpha^{-s}ds = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \Gamma(s)\zeta(s + \sigma)\alpha^{-s}ds, \tag{B.4.7}$$

where c is positive.

In the situation of our interest, σ is positive but not an integer. For instance, $\sigma = 3/2$ for particle density, and $\sigma = 5/2$ for internal energy. To evaluate the integral of the inverse Mellin transformation, we choose a contour in Figure B.1. According to the complex residue theorem, we must find the poles of the function $\Gamma(s)\zeta(s + \sigma)$ in the region

$$\Re\{s\} < c.$$

We observe that the Riemann zeta function $\zeta(t)$ has a simple pole at $t = 1$, with residue 1, and the gamma function $\Gamma(s)$ has simple poles at $s = 0$ or $s = -n$, where n is a positive integer, with residue $(-1)^n/n!$.

The Bose–Einstein integral function can thus be expanded near $z \cong 1$ as

$$g_\sigma(\alpha) = \Gamma(1 - \sigma)\alpha^{\sigma-1} + \sum_{l=0}^{\infty} \frac{(-1)^l}{l!}\zeta(\sigma - l)\alpha^l. \tag{B.4.8}$$

Worksheet B.8 Although we fail to directly obtain the Mellin transformation of the Bose–Einstein integral function, we can perform the integration term by term and deduce the trend, which gives a product of gamma and Riemann zeta functions. We plot the gamma and Riemann zeta functions, and observe the locations of poles. The `residue` command serves to find the residue of a contour integral.

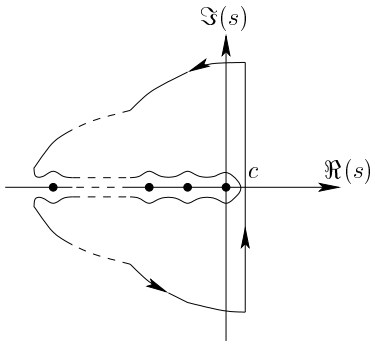


Figure B.1: Contour for evaluating the inverse Mellin transformation.

```
> assume(sigma>0);
```

```
> g := (sigma, z) -> 1/GAMMA(sigma)*int(x^(sigma-1)/(exp(x)/z - 1),
> x=0..infinity);
```

$$g := (\sigma,\, z) \to \frac{1}{\Gamma(\sigma)} \int_0^\infty \frac{x^{(\sigma-1)}}{\frac{e^x}{z} - 1}\, dx$$

```
> Eq1 := convert(taylor(g(sigma, z), z=0, 6), polynom);
```

$$Eq1 := z + \frac{z^2}{2^\sigma} + \frac{z^3}{3^\sigma} + \frac{z^4}{4^\sigma} + \frac{z^5}{5^\sigma}$$

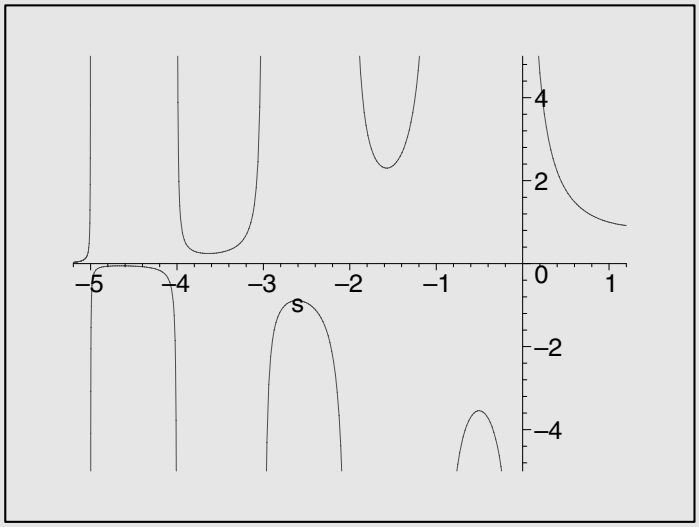
```
> Eq2 := subs(z=exp(-alpha), Eq1);
```

$$Eq2 := e^{(-\alpha)} + \frac{(e^{(-\alpha)})^2}{2^\sigma} + \frac{(e^{(-\alpha)})^3}{3^\sigma} + \frac{(e^{(-\alpha)})^4}{4^\sigma} + \frac{(e^{(-\alpha)})^5}{5^\sigma}$$

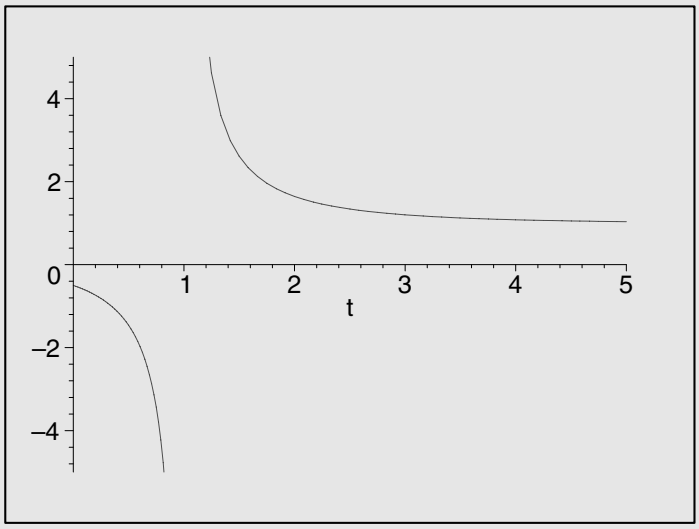
```
> Eq3 := int(Eq2*alpha^(s-1), alpha=0..infinity);
```

$$Eq3 := \Gamma(s) + 2^{(-\sigma-s)}\,\Gamma(s) + 3^{(-\sigma-s)}\,\Gamma(s) + 2^{(-2\,\sigma-2\,s)}\,\Gamma(s) + 5^{(-\sigma-s)}\,\Gamma(s)$$

```
> plot(GAMMA(s), s=-5.2..1.2, -5..5, discont=true);
```




```
> plot(Zeta(t), t=0..5, -5..5, discont=true);
```




```
> residue(Zeta(t), t=1);
```

$$1$$

```
> residue(GAMMA(s), s=0);
```

$$1$$

```
> residue(GAMMA(s), s=-1);
```

$$-1$$

```
> residue(GAMMA(s), s=-2);
```

$$\frac{1}{2}$$

```
> residue(GAMMA(s), s=-3);
```

$$\frac{-1}{6}$$

```
> residue(GAMMA(s), s=-4);
```

$$\frac{1}{24}$$

B.5 Embedding Formula

The Schwarzschild metric is

$$-ds^2 = \left(c^2 - \frac{2GM}{r}\right) dt^2 - \frac{dr^2}{1 - \dfrac{2GM}{c^2 r}} - r^2(d\theta^2 + \sin^2\theta d\phi^2). \tag{B.5.1}$$

To visualize this geometry, we use an embedding diagram, for details see Misner et al. 1973, p. 613. At one instant, a slice through $r = 0$ divides the space symmetrically into two halves; such a slice is a curved two-dimensional space. If we keep $\theta\ (= \pi/2)$, ϕ and t fixed, the metric becomes

$$ds^2 = \frac{dr^2}{1 - \dfrac{2GM}{c^2 r}}. \tag{B.5.2}$$

Because the space is curved, the ratio of the circumference to the radius is less than 2π; that is, the radius is larger than that of a flat space. To accommodate the actual radius, we introduce an artificial dimension z, so that

$$\frac{dr^2}{1 - \dfrac{2GM}{c^2 r}} = dr^2 + dz^2; \tag{B.5.3}$$

therefore,

$$dz = \pm \left(\frac{1}{1 - \dfrac{2GM}{c^2 r}} - 1 \right)^{1/2} dr.$$

The depth z is the embedding formula, which is readily solved from the integral

$$z = \int_{2GM/c^2}^{r} \left(\frac{1}{1 - \dfrac{2GM}{c^2 r'}} - 1 \right)^{1/2} dr' = \sqrt{\frac{8GM}{c^2}\left(r - \frac{2GM}{c^2}\right)}. \tag{B.5.4}$$

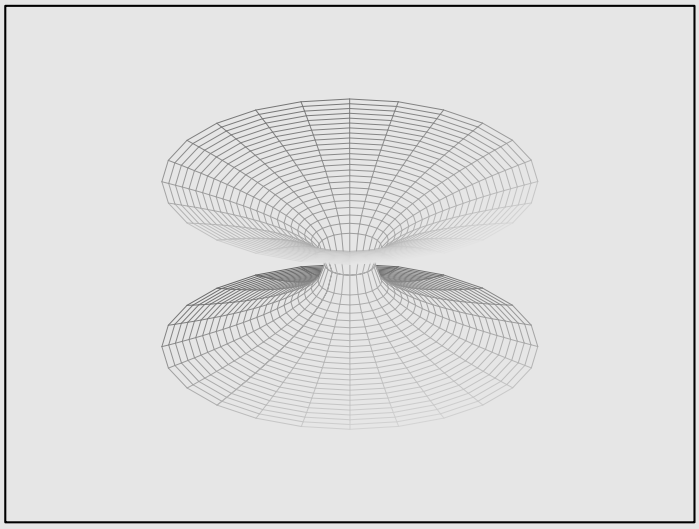
Worksheet B.9 The integral is simple. To restore the freedom in ϕ, we plot the surface of revolution of $z(r)$.

```
> z := int(sqrt(1/(1 - 2*G*M/(c^2*u)) -1), u=2*G*M/c^2..r);
```

$$z := \frac{2\sqrt{2}\sqrt{\frac{G\,M}{c^2\,r - 2\,G\,M}}\,(c^2\,r - 2\,G\,M)}{c^2}$$

```
> with(plots):

Warning, the name changecoords has been redefined
> p1 := plot3d([r*cos(phi), r*sin(phi), sqrt(8*(r-2))],
> phi=0..2*Pi, r=2..15):
> p2 := plot3d([r*cos(phi), r*sin(phi), -sqrt(8*(r-2))],
> phi=0..2*Pi, r=2..15):
> display([p1, p2], style=hidden);
```



We plot the "Schwarzschild wormhole," sometimes called the "Einstein–Rosen bridge," which connects two asymptotically flat universes together. One need not be excited about this topology: causality prevents the possibility of "time travel" using such a solution; for details, again see Misner et al. 1973, p. 837.

Exercise In 1988, Morris and Thorne devised a wormhole solution which would be stable if negative-energy material could be manufactured.[5] Their four-dimensional wormhole space

[5] M. S. Morris and K. S. Thorne, "Wormholes in spacetime and their use for interstellar travel: A tool for teaching general relativity," *American Journal of Physics*, **56**, 395–412 (1988).

time is

$$ds^2 = -e^{2\Phi}dt^2 + \frac{1}{1 - b_0^2/r^2}dr^2 + r^2(d\theta^2 + \sin^2\theta d\phi^2), \tag{B.5.5}$$

where b_0 is the radius of the throat. Find the embedding formula for this solution in the equatorial plane at a fixed time.
Answer: $z = b_0 \ln\left(r/b_0 + \sqrt{(r/b_0)^2 - 1}\right)$.

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