Course Notes for
PHYS 2502 Mathematical Physics
Spring 2022

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Preface

These are notes to accompany the Temple Physics course PHYS 2502 *Mathematical Physics.* in Spring 2022 and beyond. Prerequisites for the course are the Mathematics courses Calculus I, II, and III, and PHYS 2063 *Wave Physics.* Calculus III is the highest level course that we require in our Physics majors curriculum from the Mathematics Department. In particular, our students are not required to take courses in Differential Equations, Linear Algebra, or Complex Analysis.

I've tried hard to present things in a logical order, not relying on anything yet to come in order to introduce, or prove, something earlier on. For example, when talking about the elementary special functions, I first do the circular functions and use geometric arguments to get the derivative of $\sin(x)$, introduce the natural logarithm before introducing e^x, and then combining the circular function reasoning with e^x to come up with the hyperbolic functions. I introduce Euler's relation after doing the Taylor series for e^x, $\sin(x)$, and $\cos(x)$. Unfortunately, I haven't succeeded at this everywhere.

Nearly everything we cover in this course has either been covered in the prerequisite courses, or will be covered in required Physics courses later in the major curriculum. For the most part, the latter (which is the bulk of the material in this course) builds on the former. Therefore, my job is to reinforce the mathematics students have already seen, hopefully in a way that builds new insights, and to prepare them for their more advanced Physics courses.

I welcome feedback on these notes and the syllabus. There are far too many topics to choose from for a one-semester course. I've tried to emphasize the things that I think are most important, but opinions may differ.

A good example of this is Chapter 5 on Fourier Analysis, for which I've reserved one week (two classes). Standing waves on a stretched string, decomposed using Fourier series, were covered in Wave Physics. I will review that material, and then take the limit of an infinitely long string to derive the Fourier transform. This will also let me present the Dirac δ-function in physical context. In principle, I could take more time with this, but then something else would have to be cut down or removed entirely.

Covering Chapter 8 on Complex Analysis might be superfluous, so one might consider removing it to make room for other material. I don't think that the formalism of complex functions is needed in any of our advanced undergraduate Physics courses. However, it is indispensable when it comes to scattering theory in Quantum Mechanics, and for many problems in

Continuum Mechanics, both of which students are likely to encounter in a graduate Physics program. Unfortunately, there is nowhere else in our majors curriculum where students are likely to see this material, and it is also a particularly lovely subject, in my opinion.

As much as possible, I want to use physical examples to motivate the mathematics, but that won't be for the majority of the new material.

This course should not be the last Mathematics course you take as an undergraduate, especially if you think you are interested in pursing graduate study in Physics. You should review the offerings by the Mathematics Department and discuss options with your advisors in Physics, Mathematics, or CST. I especially recommend the course MATH 2045 *Differential Equations with Linear Algebra*. You will be very prepared for that course after taking this course. Other courses that would be particularly useful for students who want to study advanced Physics include MATH 4041 *Partial Differential Equations* and MATH 4051 *Complex Analysis*.

This course includes a laboratory, once each week, on MATHEMATICA. Those labs will only loosely parallel the material we cover in class. Mostly, I want students to come out of the lab competent to perform computer calculations that will be useful for their future coursework and research.

There are lots of good textbooks out there on "Mathematical Physics." So, why am I writing these notes? I very much wanted to try to tell a coherent story through the semester, and there is just so much material, using any outside textbook would have required me to pick and choose sections and the depth I could go to in them, and I didn't think that would be fair to the students.

However, I've found myself relying on one textbook in particular, namely "Mathematical Methods for Physics and Engineering" by Riley, Hobson, and Bence, Third Edition (2006) from Cambridge University Press, ISBN 9780521679718. It's a tome at over 1300 densely packed pages, but available in paperback for around $75. It starts out with "preliminary" material on algebra and calculus before diving into the details, and a Student's Solution Manual is available for the problems.

Course Syllabus

PHYS 2502 Mathematical Physics Spring 2022 Jim Napolitano

Wk	Ch	Day	Main Topic(s)	Key Sections
1	1	11 Jan	Fundamentals; Dimensional analysis	1.1, 1.2
		13 Jan	Derivatives and Differentials	1.3
2	1	18 Jan	Integration	1.4
		20 Jan	Elementary Special Functions	1.5
3	2	25 Jan	Taylor Series; Series as Approximations	2.1, 2.2, 2.3
		27 Jan	Euler's Formula; More than One Variable	2.4
4	3	1 Feb	First Order Ordinary Differential Equations	3.1, 3.2
		3 Feb	Second Order Equations	3.3
5	3	8 Feb	Harmonic Motion	3.4
		10 Feb	Series Solutions of Second Order Linear Equations	3.5
6	3	15 Feb	Some Important Special Functions	3.6
		17 Feb	Coupled Differential Equations	3.7
7	4	22 Feb	Vectors as Spatial Variables	4.1
		24 Feb	Vector Derivatives	4.2
8	4	8 Mar	Surface Theorems	4.3
		10 Mar	Partial Differential Equations	4.5
9	5	15 Mar	Fourier Series	5.1, 5.2, 5.3
		17 Mar	Fourier Transform	5.5
10	6	22 Mar	Vectors and Vector Spaces	6.1, 6.2
		24 Mar	Properties of Matrices	6.3
11	6	29 Mar	The Eigenvalue Problem	6.4
		31 Mar	Revisiting Coupled Oscillations	6.4.3
12	7	5 Apr	The Euler-Lagrange Equations	7.1, 7.2, 7.3
		7 Apr	Examples With Constraints	7.4
13	8	12 Apr	Complex functions and analyticity	8.2, 8.3
		14 Apr	Contour integration and residues	8.4
14	9	19 Apr	Probability Distributions	9.1, 9.2, 9.3
		21 Apr	Basic Data Analysis; Random Numbers	9.4, 9.5

Chapter 1

Basic Concepts

Mathematics is the language of Physics. According to lore, Newton invented calculus in order to explain his philosophies to weaker minds. Oliver Heaviside invented vector calculus to cast Maxwell's Equations into a form that made calculations so much easier. Eugene Wigner introduced group theory into Quantum Mechanics so that physicists had a framework for exploiting symmetry in nature.

Consequently, it is of the highest importance for students of Physics to be well versed in many different branches of Mathematics. This course should not be considered to cover "all" the Mathematics you will need, but hopefully it will introduce you to the most important concepts that you'll see later.

This first chapter is meant to cover the very basic ideas, which will lay the groundwork for the rest of the course. Most everything in this chapter is a review. But not everything.

1.1 Fundamentals

I think that one very important and simple thing to hit home, is the idea of variable names as "dummies." That is, I will use things like x, y, z, u, v, w,... a lot, but they have no physical meaning until I tell you they do. And their physical meaning will mostly be different for different problems. Also, there is often no standard terminology, so one Physics class might use a variable to mean some thing, and another class might use a different variable to mean the same thing.

1.1.1 Numbers

Used to "measure" quantities in physics. Mathematicians talk about "number fields" including integers $\mathbb{Z}$, rational numbers $\mathbb{Q}$, real numbers $\mathbb{R}$, and complex numbers $\mathbb{C}$. I will use these symbols from time to time. If I write something like $x \in \mathbb{R}$ then I mean that the variable x represents some real number.

We have some special sets of numbers. (I'll get to a more formal definition of a "set" shortly.) For example $\mathbb{R}^2$ is the set of pairs of real numbers. Physically, you can think of $\mathbb{R}^2$ as the set of points in a plane. Similarly, $\mathbb{R}^3$ is the set of real numbers in three dimensional space.

Addition, subtraction, multiplication, and division of integers, rational and real numbers are all exactly what you think they are. It is likely that you've already learned some things about the complex number system, but I'll give you some details next.

Complex numbers

The "imaginary" number i is defined as the square root of -1. That is

$$i = \sqrt{-1}$$

This makes it possible to define a "complex number" $z \in \mathbb{C}$ as

$$z = x + iy \qquad \text{where} \qquad x \in \mathbb{R}, y \in \mathbb{R}$$

(Note that $\mathbb{C}$ sounds a little like $\mathbb{R}^2$, in that there is a one-to-one correspondence through the real numbers.) We refer to x as the "real part" of z, and write $x = \Re(z)$. Similarly, y is the "imaginary part" of z, and write $y = \Im(z)$. On the blackboard, I will typically write $x = \operatorname{Re} z$ and $y = \operatorname{Im} z$, but I will always mean the same thing.

The "complex conjugate" z^* of a complex number $z = x + iy$ is

$$z^* = x - iy$$

The "modulus" of a complex number $z = x + iy$ is

$$|z| = \sqrt{(x^2 + y^2)} = (x^2 + y^2)^{1/2}$$

Addition and subtraction of complex numbers just means the addition and subtraction separately of their real and imaginary parts. Multiplication of complex numbers requires a little more care. For $z_1 = x_1 + iy_1$ and $z_2 = x_2 + iy_2$, then

$$z_1 z_2 = (x_1 + iy_1)(x_2 + iy_2) = (x_1 x_2 - y_1 y_2) + i(x_1 y_2 + x_2 y_1)$$

It is a nontrivial observation $z_1 z_2 = z_2 z_1$, namely that complex multiplication commutes. Note also that

$$z^* z = z z^* = |z|^2$$

Division of complex numbers is best understood using the modulus. For $z_1 = x_1 + iy_1$ and $z_2 = x_2 + iy_2$, we write

$$\frac{z_1}{z_2} = \frac{z_1}{z_2}\frac{z_2^*}{z_2^*} = \frac{1}{|z_2|^2} z_1 z_2^*$$

and division of complex numbers reduces to multiplication.

For more advanced manipulations of complex numbers, for example $\sqrt{z}$, it is best to wait until Section 2.4.2 when we see how to write complex numbers in terms of the modulus and a "phase" using Euler's relation.

1.1.2 Functions

A "function" maps from one number system onto itself or another number system. Mostly we will deal with functions that map real numbers onto real numbers. For example

$$f : \mathbb{R} \mapsto \mathbb{R} \qquad \text{or} \qquad u = f(x)$$

$$g : \mathbb{R}^2 \mapsto \mathbb{R} \qquad \text{or} \qquad u = g(x, y)$$

There will be many other examples, particularly when we get into vector functions. One very familiar example is the electric field from a charge distribution, which maps $\mathbb{R}^3$, that is, position in three dimensional space, onto $\mathbb{R}^3$, that is, the electric field itself.

Physicists use a wide variety of different notations, so don't get hung up on that. For example, if I write something like $f = f(x)$, all I mean is to emphasize that f is a function of the single variable x. Your intuition should be good enough to get you through anything confusing, but always ask questions if you're unsure.

1.1.3 Sets

Some collection of objects. Can be numbers, pictures, functions, i.e. anything. Denote as $\{a, b, c, \dots\}$. Examples are $\mathbb{R}$ and $\mathbb{Z}$. Subsets, eg $\mathbb{Z} \subset \mathbb{R}$. Cartesian products $\mathbb{R} \times \mathbb{R} = \mathbb{R}^2$.

Functions can in fact map from any set onto any other set, but we're not going to get that fancy in this course.

1.1.4 Groups

We can't get into it much in this course, but I want to at least introduce you to the concept of a "group." Groups are fundamental in formulating physical theory. In the same way that "numbers" measure "quantities," groups are used to measure "symmetry" in nature. One of the most common examples is the group of 3×3 real orthogonal matrices with unit determinant, which physicists write as $SO(3)$, that measures the rotational symmetry of the three dimensional world.

In order to define a group G, you need first to have two things, namely a set $\{x, y, z, \dots\}$ and a binary operation $\circ$ between elements of the set. These form a group if the following three "group axioms" are satisfied:

- There exists an identity element $\mathbb{1} \in G$ such that for any $x \in G$, $x \circ \mathbb{1} = x = \mathbb{1} \circ x$.
- For any $x \in G$ there exists an inverse element $x^{-1} \in G$ such that $x \circ x^{-1} = \mathbb{1} = x^{-1} \circ x$
- For any $x, y, z \in G$, $x \circ (y \circ z) = (x \circ y) \circ z$. That is, the binary operation is associative.

Note that there is no requirement that the binary operation be commutative, that is $x \circ y = y \circ x$. (Think about matrix multiplication, for example.) If this commutative property holds, then we say the group is "Abelian."

One simple example of a group is the real numbers $\mathbb{R}$ under addition. The identity element is zero, the inverse of any x is $-x$, and addition is clearly associative. This is also an Abelian group. The integers $\mathbb{Z}$ also form a group under addition, and in fact are a "subgroup" of $\mathbb{R}$.

A slightly more advanced group is the real numbers, excluding zero, under multiplication. Let's call that group $\mathbb{R}^*$. We have to exclude zero because if I divide any other element in the group by zero, I don't get a real number. For $x \in \mathbb{R}^*$, we see easily that $1 = \mathbb{1}$ and $x^{-1} = 1/x$. Multiplication of real numbers is obviously associative. This is also an Abelian group.

Things get more interesting when we discuss matrix operations. See Section 6.3.8.

1.2 Dimensional Analysis

Any equation has to respect the dimensions of the quantities it relates. It makes no sense to say that some number of apples is equal to some number of oranges.

By dimensions we mean the fundamental quantities that are described by the so-called base units of some system. These dimensions are length L, mass M, and time T in the most commonly used systems of units, namely SI and CGS.[1] The SI units of length, mass, and time are the meter (m), kilogram (kg), and second (s), respectively. In CGS, they are centimeter (cm), gram (g), and second (s).

Quantities that measure length, mass, or time have the dimensions L, M, and T, respectively. Derived quantities have the dimensions of the combination of fundamental quantities from which they are derived. So, for example, velocity has dimensions LT^{-1} and acceleration LT^{-2}. Force comes from mass times acceleration, so the dimensions of force are MLT^{-2}.

I will use square brackets to denote the dimensions of some quantity. So, for example, momentum $p = mv$, so $[p] = MLT^{-1}$. Angular momentum ℓ is the product of a length times momentum, so $[\ell] = ML^2T^{-1}$. Energy E is force times distance so $[E] = ML^2T^{-2}$. Notice that dimensional correctness has to carry over, so if I think of energy instead as $E = mc^2$, then its dimensions are that of mass times the square of velocity, and I get the same result.

If you do a calculation and the dimensionality of your result doesn't make sense, then you had to have made a mistake somewhere! It is always a good idea to check the dimensionality of a calculation.

Let's get the "scale" that determines the radius of a black hole, also known as the "event horizon." If you do a fancy calculation in General Relativity, which is in fact quite difficult,

[1] When it comes to electricity and magnetism, SI adds a new base unit called the Ampere, while CGS describes charges and current in units derived from mass, length and time. When we are dealing with electromagnetism in this course, I will use CGS units.

you know that in the end the event horizon R can only depend on the mass m of the black hole, the speed of light c, and Newton's gravitational constant G. So, to within factors of two and π and the like, we write

$$R = G^x m^y c^z \tag{1.1}$$

where the powers x, y, and z can be determined by dimensional analysis. The dimensions of R, m, and c are pretty obvious, namely L, M, and LT^{-1}, respectively. To get the dimensions of G, we can go back to Newton's law of gravity, namely

$$F = G\frac{m_1 m_2}{r^2} \qquad \text{so} \qquad MLT^{-2} = [G]M^2L^{-2}$$

so $[G] = M^{-1}L^3T^{-2}$. This is a handy relation to keep in mind for many problems in dimensional analysis involving gravity.

Now return to (1.1) and write

$$L = M^{-x}L^{3x}T^{-2x}M^yL^zT^{-z} = M^{-x+y}L^{3x+z}T^{-2x-z}$$

This gives us the following three equations:

$$\begin{aligned} -x + y &= 0 \\ 3x + z &= 1 \\ -2x - z &= 0 \end{aligned}$$

Adding the second and third equations gives $x = 1$. The third equation gives $z = -2$, and the first equation gives $y = 1$. Therefore, (1.1) becomes

$$R = Gm/c^2$$

A careful study of General Relativity for a static, spherical gravitating mass m yields the so-called " Schwarzschild radius" $R_S = 2Gm/c^2$ as the distance at which clocks stop. Our simple analysis, though, gets us the scale at which this happens, and in fact the right answer to within a factor of two.

1.2.1 Dimensional analysis as vector addition

Taking the logs and treating logs of units as "directions" in some space. Maybe a good first glimpse at how vector spaces can be abstracted.

1.3 Derivative of a Function of Real Variables

You probably first heard about the derivative of a function graphically, namely the slope of a line tangent to some curve at some point. Physically, the derivative tells you how something

changes. It's the same thing as the slope of a tangent line, which tells you how fast the curve is changing. In mechanics, you first see the derivative as how fast position changes with time, called the velocity, and how fast velocity changes with time, called the acceleration.

I will use generic variables to talk about the concept of a derivative, and also integration. Remember, though, these are just dummy variables. So if I write something like $y = f(x)$ and take the derivative with respect to x, I can just change the names later and talk about $x = f(t)$ to describe the position as a function of time.

1.3.1 Functions of a single variable

The derivative a function $y = f(x)$ is defined to be

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} \tag{1.2}$$

Note that the right side of the equation looks like the division of zero by zero. Indeed, the derivative is the ratio of "infinitesimal" quantities. Indeed, we often use the notation

$$f'(x) = \frac{dy}{dx}$$

Let's use this definition to find the derivative of $f(x) = x^n$ where n is a positive integer, i.e. $n = 1, 2, 3, \ldots$. Think first about the quantity

$$(x + \Delta x)^n = x^n + nx^{n-1}\Delta x + \cdots$$

where the terms I didn't write all have powers of $(\Delta x)^2$ or greater. Therefore

$$f'(x) = \lim_{\Delta x \to 0} \frac{x^n + nx^{n-1}\Delta x + \cdots - x^n}{\Delta x} = \lim_{\Delta x \to 0} \left(nx^{n-1} + \cdots \right) = nx^{n-1}$$

because the terms I didn't write down all have factors of Δx in them, so they go to zero in the limit.

So, we have proven that $f'(x) = nx^{n-1}$ for $f(x) = x^n$ where n is a positive integer. In fact, you have a homework problem to go through some steps and argue that $f'(x) = \alpha x^{\alpha-1}$ where α is any real number. It's also true if α is any complex number, but we'll leave that proof for a later time.

We will stop here for now. We will learn the derivatives of so-called "special function" when we encounter them in Section 1.5, but we have already gotten very far. For example, it is trivial to prove from (1.2) that, for constants a and b,

$$h'(x) = af'(x) + bg'(x) \qquad \text{where} \qquad h(x) = af(x) + bg(x)$$

which means that we already know how to take the derivative of a polynomial function

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots = \sum_{i=0}^{n} a_i x^i \tag{1.3}$$

and we'll see in Section 2.2 that most functions can be expressed this way if we let $n \to \infty$.

1.3.2 Differentials

When we write $f'(x) = dy/dx$ for $y = f(x)$, (1.2) tells us that dy and dx are *infinitesimal* quantities, called "differentials," which can be as small as they need to be. That is, we can ignore them if they are added to anything other than zero, and only the lowest order matters otherwise. For example, something like $dx + dx\,dy + (dx)^2$ is just the same as dx. We say that "only the lowest nonzero order is important."

Differentials are very useful for analyzing physical systems, and we will see this a lot in this course and future physics courses.

Differentials are also a very useful concept for deriving a host of mathematical relations. Consider, for example

$$d(uv) = (u + du)(v + dv) - uv = u\,dv + v\,du$$

for two functions $u = f(x)$ and $v = g(x)$. If we divide through by dx we get

$$\begin{aligned} \frac{d}{dx}(uv) &= u\frac{dv}{dx} + v\frac{du}{dx} \\ \text{or} \qquad h'(x) &= f(x)g'(x) + g(x)f'(x) \end{aligned}$$

for $h(x) = f(x)g(x)$. This is called the "product rule" for differentiation.

Now suppose instead that $h(x) = f(g(x))$, again with $u = f(x)$ and $v = g(x)$. We can derive the so-called "chain rule" for $h'(x)$ by multiplying by "1", that is

$$\begin{aligned} \frac{du}{dx} &= \frac{du}{dx}\frac{dv}{dv} = \frac{du}{dv}\frac{dv}{dx} \\ \text{or} \qquad h'(x) &= f'(g)g'(x) \end{aligned}$$

In other words, take the derivative of the function f with the function g as the argument, and then take the derivative of g with respect to x.

We can illustrate the product rule and chain rule with a simple example, namely

$$f(x) = x^n \qquad \text{and} \qquad g(x) = x^m$$

To check the product rule, let $h(x) = f(x)g(x) = x^{n+m}$. In this case we know that $h'(x) = (n + m)x^{n+m-1}$. The product rule gives

$$h'(x) = nx^{n-1}x^m + mx^n x^{m-1} = (n + m)x^{n+m-1}$$

which is correct. To check the chain rule, use $h(x) = x^{nm}$ in which case $h'(x) = nmx^{nm-1}$, but using the chain rule

$$h'(x) = \left[n\,(x^m)^{n-1}\right] mx^{m-1} = nmx^{nm-m+m-1} = nmx^{nm-1}$$

We will see plenty of more interesting examples of the produce rule and chain rule as we go through more Mathematics and Physics.

1.3.3 Higher order derivatives

We write the "second derivative" of a function $y = f(x)$ as

$$f''(x) = f^{(2)}(x) = \frac{d}{dx}\frac{dy}{dx} = \frac{d^2y}{dx^2}$$

Higher orders follow naturally, including notation.

It is worth noting that, for some reason, the Laws of Physics, including Newton's Laws, Maxwell's Equations, the Wave Equation, and many others, only involve first and second derivatives. We'll see more about this in Chapter 3 and beyond.

1.3.4 Functions of two or more variables

For a function $u = f(x, y)$ we define the "partial derivatives"

$$\frac{\partial u}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x, y) - f(x, y)}{\Delta x} \qquad \text{and} \qquad \frac{\partial u}{\partial y} = \lim_{\Delta y \to 0} \frac{f(x, y + \Delta y) - f(x, y)}{\Delta y}$$

That is, we treat $y(x)$ as a constant when we take the partial derivative withe respect to $x(y)$. For more than two variables, for example $u = f(x, y, z)$, the analogy is straightforward.

The product rule and chain rule for partial derivatives follow logically.

We will almost always only be dealing with functions where the partial derivatives commute, that is

$$\frac{\partial^2 u}{\partial x \partial y} = \frac{\partial}{\partial x}\frac{\partial u}{\partial y} = \frac{\partial}{\partial y}\frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial y \partial x}$$

1.3.5 Finding minima and maxima

A very common application of differentiation is to find maximum or minimum values of some function, and the values of the independent variable(s) that give you those extrema. More formally, for $a \leq x \leq b$, what value of x minimizes or maximizes the function $f(x)$? The generalization to functions of more than one variable is obvious.

It is of course possible that $f(a)$ and/or $f(b)$ are maximum or minimum values. If that's not the case, however, then for some value $x = x_0$ in between, $f'(x_0)$ will be positive (negative) for x slightly smaller than x_0, and negative (positive) if slightly larger, in which case $x = x_0$ is a minimum (maximum). It will often be the case that a function is defined with some "free parameters" and we need to find the derivatives with respect to these parameters and set them to zero. Solving the resulting equations gives us the values of the parameters that we're looking for.

We will see many examples of this kind of thinking.

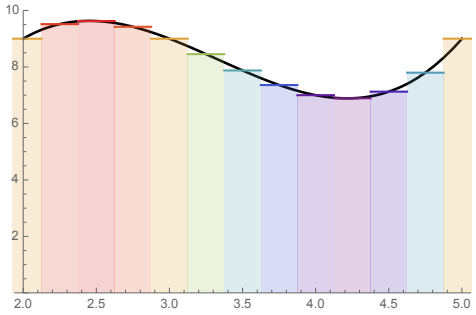


Figure 1.1: The area under a curve, approximated as the sum of a bunch of tall, rectangular boxes. The definite integral is obtained by letting the number N of boxes go to infinity, with the width Δx of each box approaching zero. This gives you a precise result for the area under the curve.

1.4 Integration

It is tempting to think of integration as the opposite of differentiation, but you should avoid the temptation.

Integration is the sum of a bunch of very small things, technically the infinite sum of infinitesimal things. It is not an accident that the integration sign $\int$ looks like a stretched out S, for "sum."

The reason you might think of integration and differentiation as opposites is because they are connected through the concept of an "antiderivative" and the Fundamental Theorem of Integral Calculus. Our goal in this sections is to connect these ideas.

1.4.1 The definite integral

The "definite" integral is an infinite sum of infinitesimal quantities. (That's the reason the integral sign looks like a tall stretched-out "S", for "Sum".) We start with an ordered set of N real numbers

$$x_i \in \{x_0, x_1, x_2, \ldots, x_N\} \tag{1.4}$$

where $a \leq x_i \leq b$. We then write

$$\int_a^b f(x)\,dx = \lim_{\substack{N\to\infty \\ \Delta x_i \to 0}} \sum_{i=0}^{N} f(x_i)\,\Delta x_i$$

where $x_1 \to a$, $x_N \to b$, and the $\Delta x_i = x_{i+1} - x_i$. The classic picture of the definite integral is "area under a curve." See Figure 1.1. A simple approximation to the area is the sum of large number of narrow vertical rectangular boxes, and the approximation becomes exact in the limits $N \to \infty$ with $\Delta x \to 0$. This is fine, and is a nice physical description, but doesn't become useful until we have the fundamental theorem of integral calculus, which we will get to shortly.

When working on some problem in physics, you always want to think of the definite integral as the sum of infinitesimals, defining the infinitesimal quantities in whatever way is handiest for you. Suppose, for example, you want to know the volume of an eggplant, a vegetable with

Figure 1.2: When you slice up an eggplant into thin pieces, each piece has the shape of a circular disk. To find the volume of the eggplant, all you need to do is add the volume of the disks, each of which is πr^2, where r is the radius of the particular disk, times the thickness of the disk. The radius r is some function of the "longwise" coordinate of the eggplant, and you'll need to know what that is to carry out the integral, but the concept should be clear from this example.

a weird shape. See Figure 1.2. If z is some coordinate that measures the position along the length of the eggplant, then when you slice the eggplant into thin disks, each with thickness dz, then the volume of the eggplant is

$$V_{\text{eggplant}} = \int_{\text{bottom}}^{\text{top}} \pi r^2 \, dz \qquad \text{with} \qquad r = r(z)$$

Of course, you'll need to know what $r(z)$ is in order to carry out the calculation, but that's something you work out for the particular eggplant you're working on.

As for how you actually carry out the integral mathematically, we need to first discuss the concept of "antiderivative", and then the Fundamental Theorem of Integral Calculus.

1.4.2 The antiderivative concept

I think one reason students often get confused is because we borrow the integration symbol to define the antiderivative as an "indefinite integral." We write

$$\int f(x)dx = F(x)$$

which just means that $f(x) = F'(x) = dF/dx$, but the reason we use the "integral" symbol for this doesn't really make sense until we connect with the definite integral. We call the function $F(x)$ the "antiderivative" of the function $f(x)$. Sometimes we write

$$\int f(x)dx = F(x) + C$$

which indicates that an arbitrary constant C can always be added to the indefinite integral. We won't usually use this way of writing the antiderivative, but it will come in handy when we are integrating to find the solutions to differential equations.

A more or less obvious example of the antiderivative is

$$\int x^\alpha \, dx = \frac{1}{\alpha + 1} x^{\alpha+1}$$

This formula breaks down when $\alpha = -1$, however. So, what is the antiderivative of the function $f(x) = 1/x$? We will investigate this in Section 1.5.2.

It is important to note, however, that not all functions have an (analytic) antiderivative. We will encounter these from time to time in Physics. Sometimes we will find "tricks" for carrying out the definite integrals nevertheless, but oftentimes the integrals need to be done numerically.

1.4.3 The fundamental theorem of integral calculus

The connection between an integral and an antiderivative. As $N \to \infty$ and the $\Delta x_i \to 0$, the Δx_i become differentials dx, and the sum (1.4) becomes

$$\int_a^b f(x) \, dx = \sum_{i=0}^{\infty} f(x_i) \, dx = \sum_{i=0}^{\infty} \frac{dF(x_i)}{dx} \, dx = \sum_{i=0}^{\infty} \Delta F(x_i) = F(b) - F(a) \equiv F(x)\Big|_a^b$$

where each term $\Delta F(x_i)$ has a cancellation with the term following it, leaving only the difference between the function evaluated at the endpoints.

If the function you're trying to integrate has no analytic antiderivative, then you have to resort to numerical integration techniques. You'll get an introduction to this technique in this course in the MATHEMATICA lab.

Want to mention that integration can be used as a technique for approximating difficult sums of finite quantities. Typical when studying statistical mechanics.

1.4.4 Changing variables in integration

Oftentimes it is convenient to express your integral in terms of a different variable from what you start with, or necessary in the case of numerical integration. You can also gain physical insight in many cases by making this so-called "change of variables" in integration. Let's see how this works.

This is, basically, an application of the chain rule in reverse, and we can approach it using differentials. Suppose you are integrating a function $f(x)$ over $a \le x \le b$, but you would prefer to integrate over a variable $y = g(x)$. It will be important that the inverse of the function $g(x)$ be well defined over $a \le x \le b$, that is $x = g^{-1}(y)$ is known. If we write $c = g^{-1}(a)$ and $d = g^{-1}(b)$ then

$$\int_a^b f(x) \, dx = \int_a^b f(x) \frac{dy}{dy} \, dx = \int_a^b f(x) \frac{dx}{dy} \, dy = \int_c^d f[g^{-1}(y)] \frac{1}{g'[g^{-1}(y)]} \, dy$$

and you are now doing an integral over $c \leq y \leq d$. This will be a lot clearer when we do some examples, but let's wait until we have defined some of the elementary special functions.

1.4.5 Integration by parts

If we apply the product rule to integration, then we come up with a technique known as "integration by parts" which can be very useful for solving physical problems and gaining insight to a physical situation. Suppose the integrand $f(x)$ can be split into the product of two functions $u(x)$ and $V(x)$, that is $f(x) = u(x)V(x)$ and you want to carry out the integral

$$\int_a^b f(x)\,dx = \int_a^b u(x)V(x)\,dx$$

Now let the antiderivative of $u(x)$ be $U(x)$, that is $dU/dx = u(x)$, and let $v(x) = dV/dx$ be the derivative of $V(x)$. Then from the product rule

$$\frac{d}{dx}(UV) = \frac{dU}{dx}V + U\frac{dV}{dx} = u(x)V(x) + U(x)v(x)$$

Integrating this equation over $a \leq x \leq b$ and rearranging terms, we get

$$\int_a^b f(x)\,dx = U(x)V(x)\Big|_a^b - \int_a^b U(x)v(x)\,dx$$

and we have "traded" an integral of $u(x)V(x)$ for one of $U(x)v(x)$, which is presumably easier to carry out. In many physical situations $U(x)V(x)\Big|_a^b = U(a)V(a) - U(b)V(b)$ will vanish. It won't be uncommon to have things like $a \to \infty$ and $b \to -\infty$.

1.4.6 Integrals in higher dimensions

You probably learned about "double integrals" and "triple integrals" in your calculus classes. These are straightforward generalizations of the one-variable integral, very similar to the generalization to partial derivatives from ordinary derivatives. So, to carry out something of the form

$$\int_a^b dx \int_c^d dy\, f(x,y)$$

you just do the x- (or y-) integral first, and then do the other one. (Notice that I moved around the dx and dy so that I could easily indicate which limits go with which variable.) This form implies that you are doing the integral over the rectangular area delimited by $a \leq x \leq b$ and $c \leq y \leq d$, but of course, that doesn't need to be the case.

More typically, in your Physics classes, at least, you will see the form

$$\int_R f(x,y)\,dA$$

where R is some specification of a region in the (x, y) plane over which you are to carry out the integral. We write $dA = dxdy$ for the infinitesimal tile in the (x, y) plane. There are other ways to write this infinitesimal area element, and we'll get to that shortly.

Integrals over volume are also common in Physics, so expect to see things like

$$\int_R f(x, y, z)\, dV$$

where now R is a region in three dimensional space, and $dV = dxdydz$. In fact, of course, the integration variables don't need to be real space, and it is not uncommon to encounter things like

$$\int_R f(x_1, x_2, \ldots, x_N)\, dx_1 dx_2 \cdots dx_N$$

and take it as it comes. We'll see specific examples of this sort of thing in this course, but for sure in your more advanced Physics courses.

Always remember that an integral is a sum of a bunch of tiny things. You can write that sum in whatever way makes the integral easiest, or do it numerically if you have to.

Polar and spherical coordinates

I want to take a little detour here, because this is a good place to introduce the common way that Physicists use to work in 2D or 3D space when there is cylindrical or spherical symmetry. I won't formally introduce you to sine and cosine until the next section, but you know enough from high school to follow along what I'm doing here.

We will be discussing different ways of describing vectors in space in Section 4.1, but let's take a moment to use simple geometry to understand how to write the integrand over a planar surface in terms of so-called "polar coordinates" (r, ϕ). That is, we locate a point in space by its distance r from the origin and the angle ϕ it makes with the x-axis. See Figure 1.3. In this case, the infinitesimal area element is

$$dA = (rd\phi) \times dr = rdrd\phi$$

so we would write the integral over some region R of the plane as

$$\int_R f(r, \phi)\, rdrd\phi$$

This is particularly powerful if the function f depends only on r, and the region R is cylindrically symmetric and goes between two limits r_1 and r_2. In this case

$$\int_R f(r, \phi)\, rdrd\phi = 2\pi \int_{r_1}^{r_2} f(r)\, rdr$$

This will often be the case in physical problems of interest.

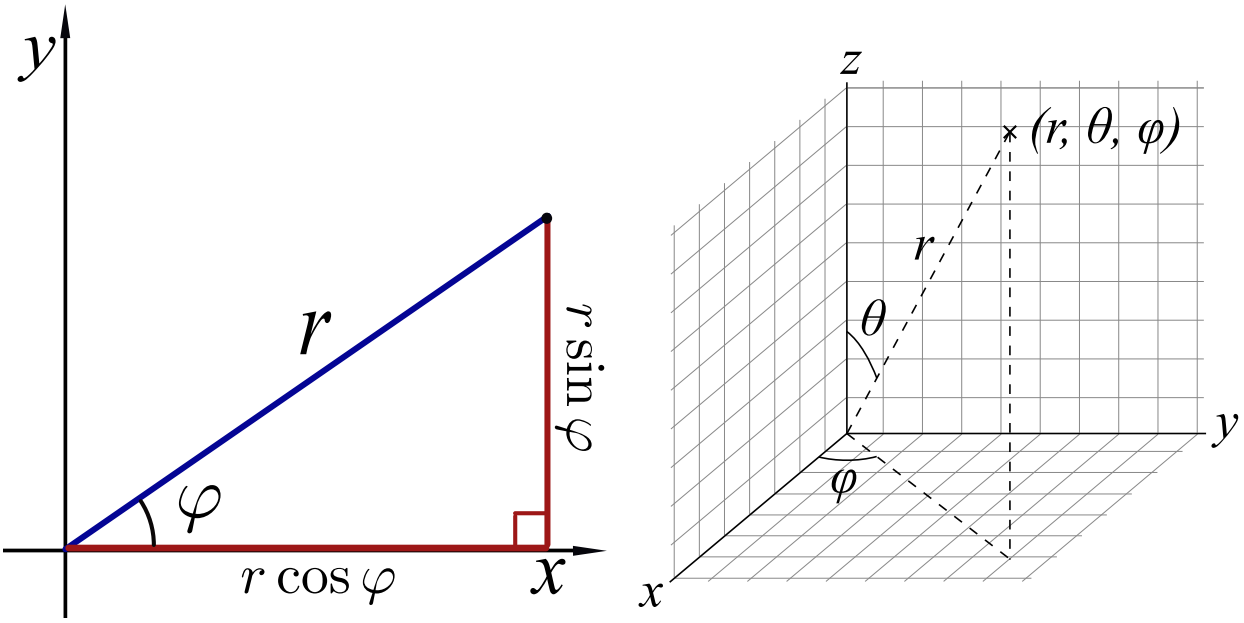


Figure 1.3: Polar and Spherical Coordinate systems with the notation commonly used in Physics. Figures taken from Wikipedia. There is no attribution given for the Polar Coordinates figure. The Spherical Coordinates figure is attributed as By Andeggs - Own work, Public Domain, https://commons.wikimedia.org/w/index.php?curid=7478049.

If we are talking about a region of three dimensional space which still has the symmetry of a cylinder, then we use the coordinates (r, ϕ, z) and treat the z-coordinate the same as usual.

Perhaps the most common three-dimensional situation in Physics is when there is spherical symmetry. In this case, we use the coordinates (r, θ, ϕ), where θ is the polar angle measured down from the z-axis. These coordinates are also illustrated in Figure 1.3. The volume element is

$$dV = (r \sin\theta \, d\phi) \times (r \, d\theta) \times (dr) = r^2 \sin\theta \, dr d\theta d\phi$$

An often useful change of variables here is $\mu = \cos\theta$, in which case the integral over a spherical volume of radius R (including $R \to \infty$) becomes

$$\int_0^R r^2 dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \, f(r, \theta, \phi) = \int_0^R r^2 dr \int_{-1}^1 d\mu \int_0^{2\pi} d\phi \, f(r, \mu, \phi)$$

where, as we'll see shortly, $d\mu = -\sin\theta \, d\theta$.

Let's illustrate this by finding the volume of a sphere. All we want to do here is add up the volume elements, so we calculate

$$\int_0^R r^2 dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi = \int_0^R r^2 dr \int_{-1}^1 d\mu \int_0^{2\pi} d\phi = \frac{R^3}{3} \times 2 \times 2\pi = \frac{4}{3}\pi R^3$$

which is something you probably remember from high school.

1.4.7 Integrals over arbitrary lines and surfaces

Always remember that an integral is a sum of a bunch of tiny things. I can't say that enough. So, we might write something like

$$\int_C f(x,y,z)d\ell$$

to denote the sum of a bunch of small things $f(x,y,z)d\ell$ along some arbitrary curve C. We'll need more information about how (x,y,z) varies along C, but that will come with the physics. If the curve C is a closed loop, then we write

$$\oint_C f(x,y,z)d\ell$$

Similarly, we can talk about integrals over some arbitrary surface S. We write

$$\int_S f(x,y,z)\,dA \to \oint_S f(x,y,z)\,dA$$

if the surface is closed. Again, we need to know a lot more about the function and the surface in order to carry out this integral.

Let's illustrate this by finding the surface area of a sphere. The area element dA in spherical coordinates is just the "inside" surface of the volume element at $r = R$, that is $dA = R^2 \sin\theta d\theta d\phi$ or $dA = Rd\mu d\phi$ for $\mu = \cos\theta$. We just sum up the surface area elements to get

$$R^2 \int_{-1}^{1} d\mu \int_0^{2\pi} d\phi = 4\pi R^2$$

which again should be something you remember from high school.

In Section 4.3 we will learn about some very important theorems that relate the integral around a closed curve to the area that the curve encloses, and the integral around a closed surface to the volume that the surface encloses. Physically, these theorems will tell us about how to learn what's "inside" from what is happening on the "boundaries."

1.5 Elementary Special Functions

Except for the little detour we took in Sections 1.4.6 and 1.4.7, the only functions we have discussed so far are power laws like x^α or their linear combination. Now it's time to more or less precisely define some common "special functions" and to study their properties.

1.5.1 Circular functions

I want to clearly define what we mean by the *functions* sine and cosine, and then make connections onto what you learned in your high school trigonometry class. See Figure 1.4.

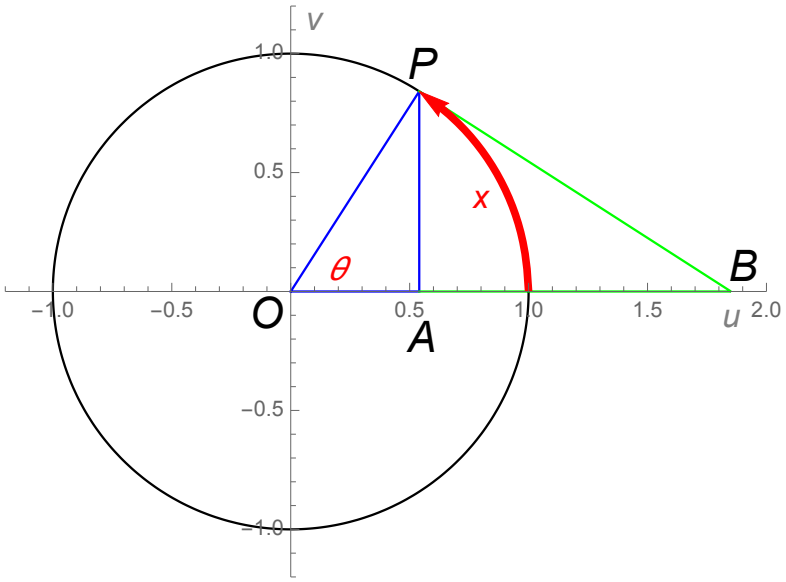


Figure 1.4: Geometry of the unit circle in the (u, v) plane. The variable x measures distance in the direction shown along the circle $u^2 + v^2 = 1$. The coordinates of the point P are defined to be $(\cos x, \sin x)$. The figure is drawn for $x = 1$. See the text for more discussion.

The cosine and sine functions are defined[2] as functions of the arc length x along a unit circle $u^2 + v^2 = 1$, counter clockwise from the point $(1, 0)$ on the (u, v) axes. That is, we define the coordinates of the point P to be $(\cos x, \sin x)$. Obviously, $\cos^2 x + \sin^2 x = 1$.

The transcendental number π is defined as the ratio of the circumference of a circle to its diameter. Therefore, the circumference of the unit circle is 2π, and if I add 2π to the argument of any circular function, I have to get the same value back. That is

$$\cos(x + 2\pi) = \cos(x) \qquad \text{and} \qquad \sin(x + 2\pi) = \sin(x)$$

and similarly for the circular functions derived from sine and cosine.

In high school, you probably learned about $\cos\theta$ and $\sin\theta$ for the right triangle OPA in Figure 1.4. If we want to talk about the angle $\theta \equiv x/R = x$ for our unit circle with radius $R = 1$, then you see that the definitions in terms of "opposite", "adjacent", and "hypotenuse" are exactly the same. Therefore, everything you learned about trigonometry in high school follows from our definition above. For example,

$$\cos\theta = \sin(\pi - \theta) = \frac{OP}{OB} = \frac{1}{OB} \qquad \text{so} \qquad OB = \frac{1}{\cos\theta} = \frac{1}{\cos x}$$

[2]The names "cosine" and "sine" seem reversed to me, also "cotangent" and "tangent." In expressions that involve both $\cos(x)$ and $\sin(x)$, I always write $\cos(x)$ first, as do most people, I think. Maybe there's an interesting story in there somewhere. However, as paraphrased from Shakespeare, "A rose by any other name would smell as sweet."

There are a bunch of useful trigonometric identities that I'm not going to bother to derive. You can look these up easily enough online, but the following are some of the most useful:

$$\cos(-x) = \cos(x) \tag{1.5a}$$
$$\sin(-x) = -\sin(x) \tag{1.5b}$$
$$\cos(x+y) = \cos x \cos y - \sin x \sin y \tag{1.5c}$$
$$\sin(x+y) = \sin x \cos y + \cos x \sin y \tag{1.5d}$$
$$\cos\frac{x}{2} = (\pm)\sqrt{\frac{1-\cos x}{2}} \tag{1.5e}$$
$$\sin\frac{x}{2} = (\pm)\sqrt{\frac{1+\cos x}{2}} \tag{1.5f}$$

You can also get many identities easily with Euler's Formula (Section 2.4), but getting there requires finding the derivatives, which we do next using the identities!

To calculate the derivative of $\cos(x)$, we go back to the fundamental definition of the derivative and make use of the identities and some geometry. We have

$$\begin{aligned}
\frac{d}{dx}\cos x &= \lim_{\Delta x\to 0}\frac{\cos(x+\Delta x)-\cos(x)}{\Delta x} \\
&= \lim_{\Delta x\to 0}\frac{\cos(x)\cos(\Delta x)-\sin(x)\sin(\Delta x)-\cos(x)}{\Delta x} \\
&= -\sin(x)\lim_{\Delta x\to 0}\frac{\sin(\Delta x)}{\Delta x} - \cos(x)\lim_{\Delta x\to 0}\frac{1-\cos\Delta x}{\Delta x}
\end{aligned}$$

The first limit can be evaluated geometrically. Refer to Figure 1.4. The area of the "slice of pie" is $(x/2\pi)\times\pi(1)^2 = x/2$, and is clearly in between the areas of right triangles OPA and OPB. It is easy to see that the area of OPA is $\cos(x)\sin(x)/2$. If we call $OP = 1$ the base of triangle OPB, then the height is

$$PB = \sqrt{OB^2 - OP^2} = \sqrt{\frac{1}{\cos^2 x} - 1} = \frac{\sin x}{\cos x}$$

and the area of triangle OPB is $\sin x/2\cos x$. Therefore

$$\frac{1}{2}\cos x\sin x < \frac{x}{2} < \frac{1}{2}\frac{\sin x}{\cos x} \qquad \text{or} \qquad \cos x \le \frac{x}{\sin x} < \frac{1}{\cos x}$$

This obviously implies that $\sin x/x \to 1$ as $x \to 0$. Now we also know that

$$\frac{1-\cos x}{x} = \frac{1-\cos x}{x}\frac{1+\cos x}{1+\cos x} = \frac{\sin x}{x}\frac{\sin x}{1+\cos x} \to (1)(0) = 0$$

as $x \to 0$. We have therefore proven that

$$\frac{d}{dx}\cos x = -\sin x$$

Given this result, it is easy to get the derivative of $\sin(x)$ from $\cos^2 x + \sin^2 x = 1$ by taking the derivative with respect to x of both sides. You find

$$\frac{d}{dx}\sin x = -\cos x$$

The derivatives of the other circular functions, like $\tan x = \cos x/\sin x$, you can get from the product rule.

I haven't discussed the inverse circular functions, that is $\cos^{-1}(x)$ and $\sin^{-1}(x)$, also known as $\arccos(x)$ and $\arcsin(x)$, but their definition and usage are pretty obvious. There is an important caveat, though, because any one value of $\sin(x)$ or $\cos(x)$ can correspond to many different values of x. For example, $\sin(\pi/4) = 1/\sqrt{2} = \sin(3\pi/4)$, so what is $\sin^{-1}(1/\sqrt{2})$? The answer is that we have a convention that the range of $y = \sin^{-1}(x)$ is $-\pi/2 \le y \le +\pi/2$, so $\sin^{-1}(1/\sqrt{2}) = \pi/4$. Similarly, the range of $y = \cos^{-1}(x)$ is $0 \le y \le \pi$.

1.5.2 Natural logarithms

I think the best way to present this is the way I learned it fifty years ago, so let's do that.

The derivative of x^n is nx^{n-1} which implies that the antiderivative exists for every function x^n except $n = -1$. So what is the function for which the derivative is $1/x$? Start by defining

$$f(x) = \int_1^x \frac{1}{t}dt$$

and show that $f(x)$ has all these properties of a logarithm.[3] For example, it is obvious that, $f(1) = 0$. Next consider, with the change of variables $u = 1/t$,

$$f\left(\frac{1}{a}\right) = \int_1^{1/a} \frac{1}{t}dt = \int_1^a u\left(-\frac{du}{u^2}\right) = -\int_1^a \frac{1}{u}du = -f(a)$$

Similarly prove (a good HW problem) that $f(ab) = f(a) + f(b)$, which implies that $f(a^n) = nf(a)$ for $n \in \mathbb{Z}^+$ (the positive integers).

So hypothesize that $f(x) = \log_b(x)$ and set about to find the base b by going back to the definition to give it the right derivative. That is

$$\begin{aligned}
\frac{d}{dx}\log_b(x) &= \lim_{\Delta x\to 0}\frac{\log_b(x+\Delta x) - \log_b(x)}{\Delta x} = \lim_{\Delta x\to 0}\frac{1}{\Delta x}\log_b\left(1+\frac{\Delta x}{x}\right) \\
&= \frac{1}{x}\lim_{\Delta x\to 0}\frac{x}{\Delta x}\log_b\left(1+\frac{\Delta x}{x}\right) = \frac{1}{x}\lim_{\Delta x\to 0}\log_b\left(1+\frac{\Delta x}{x}\right)^{x/\Delta x} \\
&= \frac{1}{x}\log_b\left[\lim_{n\to\infty}\left(1+\frac{1}{n}\right)^n\right] = \frac{1}{x}
\end{aligned}$$

[3] Maybe we need to review the definition of a logarithm, namely that $\log_b(x)$ is the function for which $b^{\log_b(x)} = x$. It should be clear from this definition that $\log_b(1) = 0$, $\log_b(b) = 1$, $\log_b(xy) = \log_b(x) + \log_b(y)$, $\log_b(1/x) = -\log_b(x)$, and $\log_b(x^\alpha) = \alpha\log_b(x)$.

This determines the value of the logarithm base b, namely

$$b = \lim_{n\to\infty} \left(1 + \frac{1}{n}\right)^n \equiv e$$

It is worth taking a few minutes to use a calculator or some app to find the value of $(1+1/n)^n$ for larger and larger values of n. One finds

$$e = 2.7182818\ldots$$

for this new transcendental number.

The function $\log_e(x) \equiv \log(x)$ is called the "natural logarithm." A lot of people write $\ln(x)$ instead of $\log(x)$, but I won't. If I ever need the logarithm to base 10, I will write $\log_{10}(x)$.

To sum things up,

$$\frac{d}{dx}\log(x) = \frac{1}{x} \qquad \text{and} \qquad \int_1^a \frac{dx}{x} = \log(a)$$

1.5.3 Exponential functions

The inverse of the natural logarithm function is called *the* exponential function. That is

$$e^{\log(x)} = x$$

which is really just the definition of the logarithm, and

$$\log(e^x) = x\log(e) = x$$

since $\log(e) = 1$, also by definition of the logarithm. An alternative notation for the exponential function is $\exp(x) = e^x$.

So what is the derivative of e^x? We answer this by using the chain rule. Writing $x = \log y$ with $y = e^x$, and taking the derivative of both sides with respect to x, we find

$$1 = \frac{1}{y}\frac{dy}{dx}$$

or $dy/dx = y$. That is

$$\frac{d}{dx}e^x = e^x$$

It is also possible to find the derivative by going back to the definition of e, but that requires an expansion using the binomial theorem, which we really won't get to until Sec. 9.3.1.

Of course, using the chain rule, putting $y = ax$,

$$\frac{d}{dx}e^{ax} = \frac{de^y}{dy}\frac{dy}{dx} = ae^{ax}$$

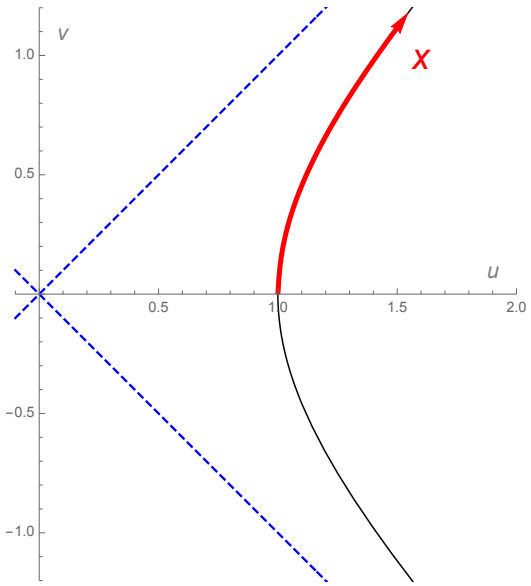


Figure 1.5: Geometry of the unit hyperbola in the (u, v) plane. The variable x measures distance in the direction shown along the hyperbola $u^2 - v^2 = 1$. The coordinates of the point at the arrow tip are defined to be $(\cosh x, \sinh x)$. The figure is drawn for $x = 1$.

1.5.4 Hyperbolic functions

There is a mistake in here that I have to fix! The analogy with circular functions and x is not in the arc length! It is with the "pie slice area" $x/2$. I will show that explicitly in here as soon as I get around to fixing this.

The circular functions $\cos x$ and $\sin x$ are defined by the coordinate values along a unit circular arc of length x. Another pair of functions, called $\cosh x$ and $\sinh x$ are defined analogously along a unit *hyperbolic* arc of length x. See Figure 1.5 and compare to Figure 1.4.

In the (u, v) plane, the unit hyperbola is $u^2 - v^2 = 1$. Therefore

$$\cosh^2 x - \sinh^2 x = 1$$

similar, but not identical to, the analogous relation for the circular functions. It's easy enough to show that $u = \cosh(x)$ and $v = \sinh(x)$ satisfy this relation with

$$\cosh(x) = \frac{e^x + e^{-x}}{2} \tag{1.6a}$$

$$\text{and} \qquad \sinh(x) = \frac{e^x - e^{-x}}{2} \tag{1.6b}$$

This also makes it simple to calculate the derivatives of the hyperbolic functions. You find

$$\frac{d}{dx}\cosh x = \sinh x \qquad \text{and} \qquad \frac{d}{dx}\sinh x = \cosh x$$

After we learn Euler's Relation in Section 2.4, we can make an analytic connection to the connection with $\cos(x)$ and $\sin(x)$.

There is actually an interesting physical connection between the circular and hyperbolic functions. The circular functions are used to generate rotations in a plane. That is, the "change coordinates" in two dimensional space from some (x, y) to a different (x', y'). In Section 6.5 we will see that the hyperbolic functions perform the same "coordinate change" in relativistic "space time", converting some (t, x) to a different (t', x').

1.5.5 The Gamma function

An important special function that we can now define and work with.

$$\Gamma(z) \equiv \int_0^\infty x^{z-1} e^{-x}\, dx \qquad z \in \mathbb{C} \;\text{ where }\; \Re(z) > 0 \tag{1.7}$$

It is a function of a complex number, but in this course we will only refer to the real numbers, in fact only use $z \in \mathbb{Z}^+$, that is the integers $z = n = 1, 2, 3 \ldots$.

The reason physicists find a lot of use for the gamma function is because it is an analytic form for the factorial, which shows up a lot in statistical mechanics and other fields. This is easy to see if we consider integrating by parts. That is

$$\Gamma(n+1) = \int_0^\infty x^n e^{-x}\, dx = \left[x^n(-e^{-x})\right]_0^\infty - \int_0^\infty n x^{n-1}(-e^{-x})\, dx = n\Gamma(n)$$

It is also pretty clear that $\Gamma(1) = 1$ is just from the definition, so repeated application of this result leads us to

$$\Gamma(n+1) = n \cdot (n-1) \cdot (n-2) \cdots (1) = n!$$

for $n \in \mathbb{Z}^+$. Notice that $\Gamma(1) = 1$ tells us that we can consistently define $0! = 1$.

1.5.6 Gaussian integrals

Physicists make a lot of use of the so-called "error function" in statistical analysis and elsewhere. Refer to Section 9.3.3 for why we see this so often, and where the name comes from. To discuss this, we first need to discuss the concept of the "Gaussian integral."

The infinite Gaussian integral

Note that the antiderivative of e^{-x^2} cannot be determined analytically. However, there is a nifty trick we can use to determine the definite integral over $-\infty \leq x \leq \infty$. We write

$$I = \int_{-\infty}^{\infty} e^{-x^2}\, dx = 2\int_0^\infty e^{-x^2}\, dx$$

where the second relation will come in handy from time to time, and is only the observation that the integrand is an even function of x. Now we obviously can also write

$$I^2 = \left[\int_{-\infty}^{\infty} e^{-x^2}\,dx\right]\left[\int_{-\infty}^{\infty} e^{-y^2}\,dy\right] = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-(x^2+y^2)}\,dxdy$$

If we interepret[4] x and y as variables in the plane, and switch instead to variables r and ϕ, as described in Section 1.4.6, we get

$$I^2 = \int_0^{2\pi} d\phi \int_0^{\infty} rdr\, e^{-r^2} = 2\pi\left[-\frac{1}{2}e^{-r^2}\right]_0^{\infty} = \pi$$

where now we realize that the integrand re^{-r^2} *does* have an analytic antiderivative! Therefore $I = \sqrt{\pi}$. The exponent function in fact usually has a slightly more complicated argument, so we write, using a change of variables $y = x\sqrt{a}$ so $dx = dy/\sqrt{a}$,

$$I(a) = \int_{-\infty}^{\infty} e^{-ax^2}dx = \int_{-\infty}^{\infty} e^{-y^2}\frac{1}{\sqrt{a}}dy = \sqrt{\frac{\pi}{a}} \tag{1.8}$$

Derivatives of the infinite Gaussian integral

We can use (1.8) to find other important integrals. For example

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2}\,dx = -\frac{d}{da}\int_{-\infty}^{\infty} e^{-ax^2}\,dx = -\frac{d}{da}I(a) = \frac{1}{2}\sqrt{\frac{\pi}{a^3}} \tag{1.9}$$

Asymptotic expansion of the Gaussian Integral

This is a good place to make students aware of the idea of an asymptotic expansion. I would use the example from Schroeder's appendix:

$$\int_x^{\infty} e^{-t^2}\,dt = e^{-x^2}\left(\frac{1}{2x} - \frac{1}{4x^3} + \frac{3}{8x^5} - \cdots\right) \qquad \text{for} \qquad x \gg 1$$

and show what happens when you go too far in the series.

Possibly better to do it before Taylor series to avoid confusion? Maybe not enough time to get this deep into this anyway.

The error function

We now have enough to define the error function, namely

$$\text{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-x^2}\,dx$$

which rises monotonically from $\text{erf}(0) = 0$ to $\text{erf}(z \to \infty) = 1$.

[4]We are actually doing a change of variables from (x, y) to (r, ϕ), but I don't want to be too technical here since we haven't gotten yet to the machinery of changing variables in more than one dimension.

1.6 Using MATHEMATICA

This course includes a laboratory section aimed at getting you to use MATHEMATICA for symbolic manipulations, plotting, and some data analysis. Exercises will include material from calculus and differential equations, and matrix operations. Although the topics will more or less parallel what we do in the lecture, the laboratory exercises are not meant to specifically reinforce the material in the homework and quizzes. That is, the MATHEMATICA lab is essentially a separate portion of the course.

It may happen that I use MATHEMATICA code in these notes to illustrate something, perhaps techniques for numerically solving differential equations, for example.

Many of the figures that I've produced for these notes come from MATHEMATICA code that I have written. Figure 2.1 is a rather simple example. Figure 1.4, on the other hand, is a bit more complicated. If you would like to see the code I used for these, or any other, figures, just let me know.

Chapter 2

Infinite Series

Infinite series appear all of the time in mathematics that is used in physics. They provide excellent ways to connect mathematical concepts and to solve differential equations. Truncated infinite series are also very important in approximations.

Most of this chapter should be review.

2.1 A Simple Power Series

Let's start with a simple example of a *finite* series, maybe the simplest thing we can think of. We write

$$S_n = 1 + x + x^2 + \cdots + x^n$$

where n is a positive integer. We call this a "power series" in x. There is a nifty trick for finding ana analytical expression for S_n. First, multiply this by x, that is

$$xS_n = x + x^2 + x^3 + \cdots + x^{n+1}$$

Subtracting the second expression from the first lets us solve for S_n, namely

$$S_n = \frac{1 - x^{n+1}}{1 - x} \tag{2.1}$$

So what happens if we let $n \to \infty$, that is, let the series become *infinite*? Well, we will get some kind of nonsense if $x \geq 1$. If $x = 1$, then (2.1) gives $0/0$, and if $x > 1$ then it gives ∞. Similar problems come in if we have $x \leq -1$. It seems that to make sense of the case for $n \to \infty$, then, we must require that $-1 < x < 1$, or $|x| < 1$. In this case, we have, for $x \in \mathbb{R}$,

$$\frac{1}{1 - x} = 1 + x + x^2 + x^3 + \cdots \qquad \text{where} \qquad |x| < 1 \tag{2.2}$$

This is our first example of an infinite series, and we will see it very often in physics. (In fact, it is a specific case of another example we'll see shortly.) If we put $x \to -x$, then

$$\frac{1}{1+x} = 1 - x + x^2 - x^3 + \cdots \qquad \text{where} \qquad |x| < 1$$

In the case that $|x| \ll 1$, we come up with a very important approximation, namely

$$\frac{1}{1 \pm x} = 1 \mp x + \mathcal{O}(x^2)$$

which we'll use over and over again in physics. The term $\mathcal{O}(x^2)$ means "of order x^2", and is an important notation when we want to estimate how close the approximation is to the truth.

We'll go through these same notions in the rest of this chapter, but in the more general "Taylor Series" which we can apply to functions as a rule.

2.1.1 Convergence of the power series

Somehow I think it would be a good idea to discuss the idea of convergence, more than the little bit I discussed above. I have to think about what I would say, though. Maybe let $x \to z$, a complex number, and talk about convergence in the complex plane?

2.2 Taylor Series

Instead of deriving the idea of Taylor Series step by step, I think it is better to give you the answer first, discuss it using some graphics, and then go on to show you how you get there.

Taylor's theorem, which we will (more or less) prove shortly, says that for any function $f(x)$ for which derivatives at a point $x = x_0$ are well defined, we can write

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2!}f''(x - x_0)^2 + \cdots = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(x_0)(x - x_0)^n \qquad (2.3)$$

where $f^{(n)}(x_0)$ is a shorthand for the nth derivative evaluated at $x = x_0$, that is

$$f^{(n)}(x_0) = \left. \frac{d^n}{dx^n} f(x) \right|_{x=x_0}$$

In other words, pretty much any function can be written as a (possibly) infinite polynomial in the variable $x - x_0$, and this polynomial can be written analytically to any order given an analytic expression for $f(x)$. We will encounter later some "special functions" (like Bessel's function, spherical Bessel functions, ...) which only can be written as Taylor series, but let's not dwell on that for now.

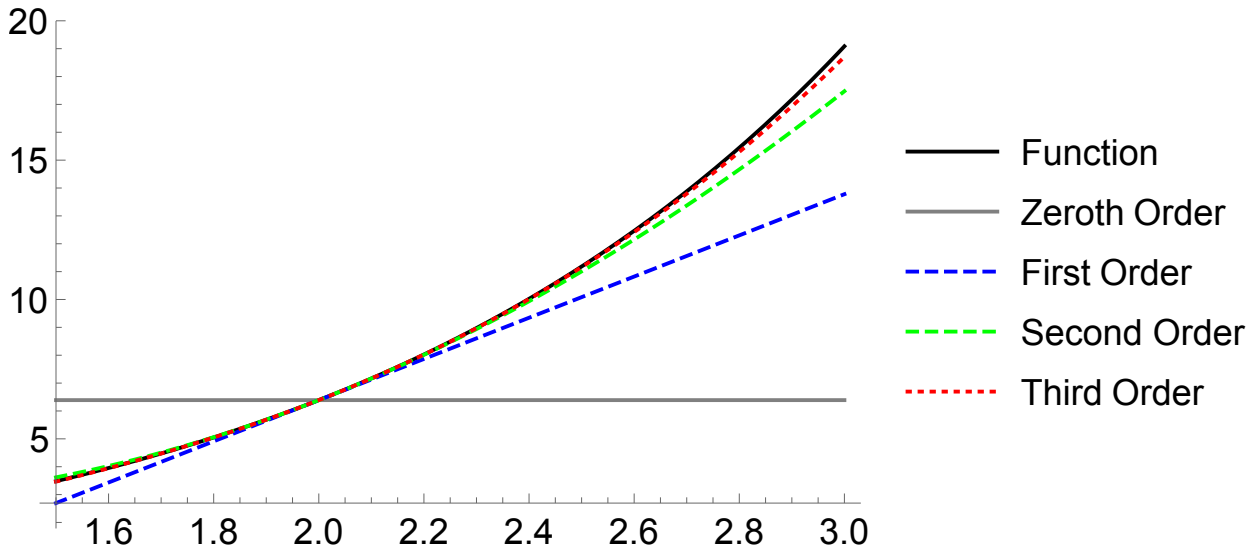


Figure 2.1: Graphic demonstration of a Taylor series expansion. This example expands the function, plotted as a black solid line, about the point at $x_0 = 2$, up to third order.

It is not necessary for $x \in \mathbb{R}$, but in this course, this is the only case we will study seriously. Expansions of complex functions in terms of complex variables are especially important in many advanced physics courses.

Equation (2.3) may look like a mouthful, but it is actually quite easy to interpret. Look at the first two terms. Ignoring the others gives

$$f'(x_0) = \frac{f(x) - f(x_0)}{x - x_0}$$

which says that $f'(x_0)$ is the slope of the straight line that passes through $x = x_0$. In other words, the first two terms are a "straight line" approximation to $f(x)$. Adding higher terms just makes higher order approximations. Figure 2.1 shows pretty clearly, I think, how the Taylor expansion terms represent a systematic better and better approximation to the function, especially as $|x - x_0| \ll 1$. This is also the idea behind using Taylor expansions as approximations.

Now let's move on to see where (2.3) comes from.

2.2.1 Expanding about $x = 0$

.

The easiest path to deriving (2.3) is to start with $x_0 = 0$. Assume that we can write

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots$$

and see how we might find the coefficients a_n. This is actually pretty simple, since

$$\begin{aligned} f(0) &= a_0 \\ f'(0) &= 1 \cdot a_1 \\ f''(0) &= 2 \cdot 1 \cdot a_2 \\ f'''(0) &= 3 \cdot 2 \cdot 1 \cdot a_3 \end{aligned}$$

and so forth. In other words, $f^{(n)}(0) = n! \cdot a_n$, and so

$$f(x) = f(0) + f'(0)x + \frac{1}{2!}f''(0)x^2 + \cdots = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0) x^n \tag{2.4}$$

Remember that 0!=1. If you don't believe me, review Section 1.5.5 and find $\Gamma(1)$.

Let's use this approach to derive the Taylor expansion for $f(x) = 1/(1-x)$, that is (2.2). All we need to do is calculate $f(x)$ and its derivatives at $x = 0$.

$$f(0) = 1 \qquad f'(0) = -(-)\left.\frac{1}{(1-x)^2}\right|_{x=0} = 1 \qquad f''(0) = -2(-)\left.\frac{1}{(1-x)^3}\right|_{x=0} = 2$$

and so forth. In other words, $f^{(n)}(0) = n!$ and we get (2.2).

2.2.2 Simple examples

Let's derive the Taylor expansions (about $x = 0$)[1] for some of the functions from Section 1.5. The simplest is for $f(x) = e^x$, since the derivative of e^x is just e^x so that $f^{(n)}(0) = 1$ for all n, and

$$e^x = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots \tag{2.5}$$

This result is used so often in physics that you should memorize it.

The expansions for $\cos(x)$ and $\sin(x)$ are also pretty easy. The derivative of $\cos(x)$ is $-\sin(x)$ and the derivative of $\sin(x)$ is $\cos(x)$. Also, of course, $\cos(0) = 1$ and $\sin(0) = 0$. The series expansions therefore are only the terms that have $\cos(x)$ as the derivative, with alternating signs. You find

$$\cos x = 1 - \frac{1}{2!}x^2 + \frac{1}{4!}x^4 + \cdots \tag{2.6a}$$

$$\sin x = x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 + \cdots \tag{2.6b}$$

The expansion for $f(x) = \log(1+x)$ is more interesting. In the first place, we consider this instead of $f(x) = \log(x)$ because $f(0)$ would not be defined in this case. The derivatives are straightforward, namely

$$f'(x) = \frac{1}{1+x} \qquad f''(x) = -\frac{1}{(1+x)^2} \qquad f'''(x) = -2\frac{1}{(1+x)^3}$$

[1] I think that Taylor expansions about $x = 0$ are called "Maclaurin expansions."

which brings us to $f^{(n)}(0) = -(-1)^n(n-1)!$ for $n \geq 1$, and $f(0) = \log 1 = 0$. Therefore

$$\log(1+x) = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 + \cdots \tag{2.7}$$

This is also a formula that you will see often in physics problems.

Another very common expansion in physics is for functions of the form $f(x) = (1+x)^\alpha$, where $\alpha \in \mathbb{R}$. You should take the time to work out the first few terms of the expansion yourself. (You might also try using the Series function in MATHEMATICA to find the expansion.) The result is

$$(1+x)^\alpha = 1 + \alpha x + \frac{1}{2}(\alpha-1)\alpha x^2 + \frac{1}{6}(\alpha-2)(\alpha-1)\alpha x^3 + \cdots \tag{2.8}$$

It should also become second nature to you to think that $(1+x)^\alpha = 1 + \alpha x$ when $|x| \ll 1$.

2.2.3 Expanding about $x = x_0$

Now let's return to deriving (2.3). Start with (2.4) and change variables to $y = x + x_0$. Clearly, the derivative with respect to y is the same as the derivative with respect to x, since $dy/dx = 1$. Setting $x = 0$ is the same as setting $y = y_0$. Therefore, (2.4) becomes

$$f(y) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(x_0)(y - x_0)^n$$

Then just write $y \to x$ and you recover (2.3) and we're done.

As an example, let's expand $f(y) = \log(y)$ about $y = 1$ and compare to (2.7). Since

$$f'(y) = \frac{1}{y} \qquad f''(y) = -\frac{1}{y^2} \qquad f'''(y) = 2\frac{1}{y^3}$$

and so on, we have $f(1) = 0$, $f'(1) = -1$, $f''(1) = 2$, etc.... Therefore we end up with

$$\log(y) = (y-1) - \frac{1}{2}(y-1)^2 + \frac{1}{3}(y-1)^3 + \cdots$$

Switching to $x = y - 1$ recovers (2.7).

2.3 Expansions as Approximations

Physicists make a lot of use of (2.3) and (2.4) in approximations. So long as $|x| \ll 1$ in (2.4), or $|x - x_0| \ll 1$ in (2.3), the successive terms in the expansion will be smaller and smaller as the order increases. It is therefore likely that the first term or two or three will be plenty good enough for your application.

We refer to approximation schemes like this as "expanding in some small parameter." Oftentimes, though, the quantity x, or $x - x_0$, will have dimensions, so we need to know that

it is small compared to something else? *The best approach here is always to express your formula in terms of a dimensionless parameter before expanding.*

We can illustrate this with a cute physics problem. We refer to the acceleration of gravity near the Earth's surface as g, a number likely ingrained in your memory as $g = 9.8$ m/s^2. We treat g as a constant for the motion of falling bodies, projectiles, and the like. However, since the force of gravity decreases as we move out from the center of the Earth, we expect g to actually be a function of the height y above the Earth's surface. The dependence on y should be very weak, since any change in height would be much smaller than the Earth's radius R, but it could be important if we are making a precise measurement of the motion.

So how can we get a useful approximation for $g(y)$ that is good for $y \ll R$? The force of gravity on an object of mass m that is a distance $r = R + y$ from the center of the Earth is

$$F_{\rm grav} = G\frac{mM}{r^2} = G\frac{mM}{(R+y)^2} = mg$$

where M is the mass of the Earth. Therefore

$$g(y) = \frac{GM}{(R+y)^2} = \frac{GM}{R^2}\left(1 + \frac{y}{R}\right)^{-2}$$

This formula is "exact" (for a spherical Earth of uniform density), but its form makes it difficult to solve differential equations for the motion of objects. On the other hand, I have written this formula in terms of a small parameter $y/R \equiv x$, and can make use of the expansion (2.8) to simplify it. We have

$$g(y) \approx \frac{GM}{R^2}\left(1 - 2\frac{y}{R}\right) = g_0(1 - \beta y)$$

where $g_0 = gM/R^2 = 9.8$ m/s^2 and $\beta = 2/R = 3.1 \times 10^{-7}$/m. In other words, near the Earth's surface, the acceleration due to gravity decreases linearly with height, by a fractional amount of 3.1×10^{-5} per 100 m.

2.4 Euler's Formula

We are now in a position to derive one of the most important and useful formulas in physics. You will use this result, called "Euler's Formula", in almost every physics course you take.

Consider the expansion about $x = 0$ for e^x given by (2.5). Now instead of expanding the function e^x, expand the function $f(x) = e^{ix}$. Since $i^2 = -1$, we know that $i^3 = -i$, $i^4 = 1$, $i^5 = i$,and so on. That is, $i^n = \pm i$ for n odd, and $i^n = \pm 1$ for n even. This gives

$$\begin{aligned} e^{ix} &= 1 + ix - \frac{1}{2!}x^2 - i\frac{1}{3!}x^3 + x^4\frac{1}{4!}x^4 + i\frac{1}{5!}x^5 + \cdots \\ &= 1 + -\frac{1}{2!}x^2 + \frac{1}{4!}x^4 + \cdots \\ &\quad + i\left(x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 + \cdots\right) \end{aligned}$$

We recognize the two expansions above from (2.6) and arrive at Euler's Formula:

$$e^{ix} = \cos x + i \sin x \tag{2.9}$$

One of the first places we use Euler's Formula is in oscillations, where instead of writing $\cos \omega t$ and $\sin \omega t$ we'll find it much handier to write $e^{\pm i\omega t}$.

Turning Euler's Formula around gives us

$$\cos x = \frac{e^{ix} + e^{-ix}}{2} \tag{2.10a}$$

$$\text{and} \qquad \sin x = \frac{e^{ix} - e^{-ix}}{2i} \tag{2.10b}$$

which bear a striking resemblance to (1.6). In fact, we see that

$$\cosh(ix) = \cos(x) \qquad \text{and} \qquad \sinh(ix) = i \sin(x)$$

2.4.1 Trigonometric identities

Euler's Formula makes it easy to find various trigonometric identities. For example, writing $e^{i(x+y} = e^{ix}e^{iy}$ becomes

$$\begin{aligned} \cos(x+y) + i\sin(x+y) &= (\cos x + i \sin x)(\cos y + i \sin y) \\ &= \cos x \cos y - \sin x \sin y + i(\sin x \cos y + \cos x \sin y) \end{aligned}$$

Just equate real and imaginary parts to get (1.5c) and (1.5d).

I don't think it is fair to call these "derivations" because in order to get Euler's Formula, I needed to know how to find the derivatives of $\cos x$ and $\sin x$, and I got these by using the trigonometric identity for the cosine of the sum. Nevertheless, this is a useful technique for finding more identities, or at least figuring them out if you need them and can't look them up easily.

2.4.2 Polar representation of complex numbers

Euler's Formula gives us a very useful way to express complex numbers in a polar form.

See Figure 2.2. The point in the complex plane can be identified either by its Cartesian coordinates (x, y), or by its polar coordinates (r, ϕ). That is, we can write $z = x + iy$ as $z = re^{i\phi} = r\cos\phi + ir\sin\phi$ since $x = r\cos\phi$ and $y = r\sin\phi$.

We call $r = (x^2 + y^2)^{1/2}$ the *ampltiude* and $\phi = \tan^{-1}(y/x)$ the *phase* of the complex number z. This terminology gains physical importance when we apply it to the amplitude and phase of an oscillating system. See Section 3.4.

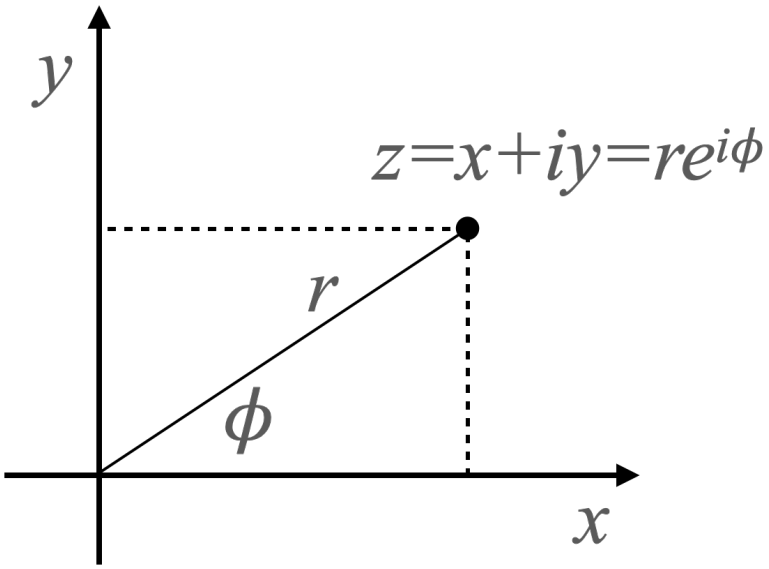


Figure 2.2: Polar representation of a complex number.

2.4.3 Application: Simple Harmonic Motion

This is a good time to make use of Euler's formula to solve a basic and crucially important problem in elementary mechanics, namely Simple Harmonic Motion. It is also an opportunity to introduce the material on Ordinary Differential Equations that is the focus of Chapter 3.

Figure 2.3 shows the physical situation. A mass m is attached to a spring with stiffness k, and can slide without friction on a horizontal surface. There is a restoring force $F = -kx$ acting on the mass. The (horizontal) acceleration of the mass is $\ddot{x}(t) = d^2x/dt^2$. Newton's Second Law "$F = ma$" tell us that the force must equal the mass times the acceleration, so

$$-kx = m\frac{d^2x}{dt^2} \qquad \text{or} \qquad \frac{d^2x}{dt^2} = -\omega_0^2 x(t) \qquad \text{where} \qquad \omega_0^2 \equiv \frac{k}{m} \tag{2.11}$$

Equation (2.11) is a *differential equation* that would be solved for the motion $x(t)$, that is, the function $x(t)$ that maps time onto position.

Euler's formula gives us an elegant way to find the solution $x(t)$ to (2.11). In words, we need to find a function that, when you take its derivative *twice*, returns the same function but multiplied by $-\omega_0^2$. You know that the derivative with respect to x of a function $f(x) = e^{ax}$ is just $f'(x) = ae^{ax}$. Therefore, the derivative with respect to t of $e^{i\omega_0 t}$ is $i\omega_0 e^{i\omega_0 t}$, and taking the derivative a second time just brings down another factor of $i\omega_0$. That is

$$\frac{d^2}{dt^2}e^{i\omega_0 t} = (i\omega_0)^2 e^{i\omega_0 t} = -\omega_0^2 e^{i\omega_0 t}$$

which is just what we wanted!

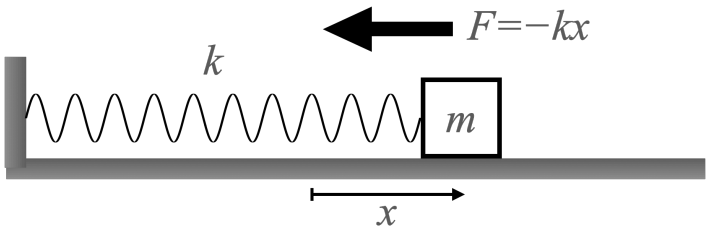


Figure 2.3: The physical situation leading to simple harmonic oscillation. The variable $x = x(t)$ measures the position of the mass m relative to the equilibrium point at $x = 0$. The "restoring force" $F = -kx$ wants to pull the mass back to the equilibrium position.

However, there is also a second choice, namely

$$\frac{d^2}{dt^2}e^{-i\omega_0 t} = (-i\omega_0)^2 e^{-i\omega_0 t} = -\omega_0^2 e^{-i\omega_0 t}$$

So, how do we deal with the fact that there are two different solutions $x(t)$ to the differential equation?

In fact, we'll find in Chapter 3 that any differential equation with a second derivative will end up having two possible solutions. We'll also learn that, in fact, there are an *infinite* number of solutions for this kind of differential equation, called a *linear* differential equation because the function $x(t)$ and its derivatives only appear in linear form. There are an infinite number of solutions because any linear combination of the two different "independent" solutions is also a solution. That is, the general solution to (2.11) is

$$x(t) = Ae^{i\omega_0 t} + Be^{-i\omega_0 t} \tag{2.12}$$

where A and B are arbitrary constants. We can see this explicitly just by taking the second derivative. That is,

$$\frac{d^2}{dt^2}(A^{i\omega_0 t} + Be^{-i\omega_0 t}) = -\omega_0^2 A^{i\omega_0 t} - \omega_0^2 Be^{-i\omega_0 t} = -\omega_0^2(A^{i\omega_0 t} + Be^{-i\omega_0 t})$$

Now our question is how do we find the constants A and B. For this, we put in the physics of the so-called "initial conditions." Where is the mass m at $t = 0$, and how fast, and in what direction, is it going at this point? Let's say the initial position is x_0. Then

$$x(0) = A + B = x_0$$

We get a second equation for A and B by considering the velocity, that is

$$v(t) = \dot{x}(t) = \frac{dx}{dt} = i\omega_0 A^{i\omega_0 t} - i\omega_0 Be^{-i\omega_0 t}$$

If the initial velocity is v_0, then

$$v(0) = i\omega_0 A - i\omega_0 B = v_0 \qquad \text{or} \qquad A - B = \frac{v_0}{i\omega_0}$$

We now have two equations to solve for A and B in terms of the physical initial values of position and velocity, x_0 and v_0. The equations are simple to solve. You find

$$A = \frac{1}{2}\left(x_0 - i\frac{v_0}{\omega_0}\right) \qquad \text{and} \qquad B = \frac{1}{2}\left(x_0 + i\frac{v_0}{\omega_0}\right)$$

(Notice that $B = A^*$. This will become handy shortly.) We can now write down the solution $x(t)$ that satisfies the differential equation and also the initial conditions:

$$\begin{aligned} x(t) &= Ae^{i\omega_0 t} + Be^{-i\omega_0 t} \\ &= \frac{1}{2}\left(x_0 - i\frac{v_0}{\omega_0}\right)(\cos\omega_0 t + \sin\omega_0 t) + \frac{1}{2}\left(x_0 + i\frac{v_0}{\omega_0}\right)(\cos\omega_0 t - \sin\omega_0 t) \\ &= x_0\cos\omega_0 t + \frac{v_0}{\omega_0}\sin\omega_0 t \end{aligned} \tag{2.13}$$

(Notice how the i magically disappears, but it had to; $x(t)$ is a real function with real initial conditions.) You should convince yourself that this solves the differential equation (2.11), and satisfies the initial conditions.

We can also use Euler's formula to write the solution in an alternate form, which gives some physical insight into what's going on. Since $B = A^*$, we can write

$$A = \frac{1}{2}Re^{i\phi} \qquad \text{and} \qquad B = \frac{1}{2}Re^{-i\phi}$$

where R and ϕ are related to the initial conditions through

$$R = \left(x_0^2 + \frac{v_0^2}{\omega_0^2}\right)^{1/2} \qquad \text{and} \qquad \phi = -\tan^{-1}\left(\frac{v_0}{\omega_0 x_0}\right) \tag{2.14}$$

In this case, we write our solution as

$$\begin{aligned} x(t) &= Ae^{i\omega_0 t} + Be^{-i\omega_0 t} \\ &= \frac{1}{2}R^{i\phi}e^{i\omega_0 t} + \frac{1}{2}Re^{-i\phi}e^{-i\omega_0 t} \\ &= \frac{1}{2}R\left[e^{i(\omega_0 t+\phi)} + e^{-i(\omega_0 t+\phi)}\right] \\ &= R\cos(\omega_0 t + \phi) \end{aligned} \tag{2.15}$$

We call R the "amplitude" of the oscillation; it is the maximum value that $x(t)$ can reach, so the mass m moves between $+R$ and $-R$. The (angular) frequency of the oscillation is ω_0, so the period is $T = 2\pi/\omega_0$. The phase ϕ measures the "time lag" of the oscillation. If $v_0 = 0$, then $\phi = 0$ and the mass starts at the maximum value; it's as if you pull the mass and let it go (from rest) at $t = 0$. If the initial position $x_0 = 0$, however, then $\phi = -\pi/2$, and the motion starts a quarter period "behind."

Figure 2.4 shows three curves of $x(t)$ for three different choices of initial conditions. Each

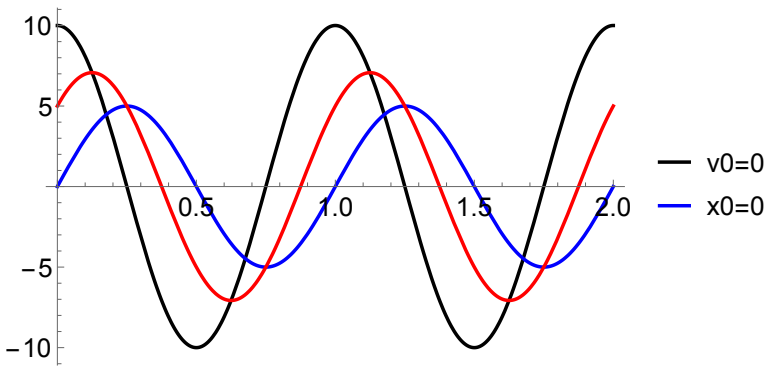


Figure 2.4: Simple harmonic motion with different combinations of initial position and velocity, corresponding to different amplitudes and phases. The red curve is for zero initial velocity, the blue curve is for zero initial position, and the red curve is for neither of the two are zero. See the text for details.

curve is drawn for $\omega_0 = 2\pi$, that is oscillation period $T = 1$. The black curve uses $x_0 = 10$ and $v_0 = 0$, while the blue curve is plotted for $x_0 = 0$ and $v_0 = 5\omega_0$. Notice that the blue curve lags the black curve by a quarter of a period, as expected given that their relative phases are $\pi/2$. The red curve corresponds to $x_0 = 5$ and $v_0 = 5\omega_0$, and appropriately lags by a phase of $\pi/4$.

2.5 Expansions in More than One Variable

From time to time, it will be useful to perform Taylor expansions in functions of more than one variable. The generalization is straightforward. Up to second order, for a function of two variables, you find

$$\begin{aligned} f(x,y) &= f(x_0,y_0) + \left.\frac{\partial f}{\partial x}\right|_{x=x_0,y=y_0}(x-x_0) + \left.\frac{\partial f}{\partial y}\right|_{x=x_0,y=y_0}(y-y_0) \\ &\quad + \frac{1}{2!}\left.\frac{\partial^2 f}{\partial x^2}\right|_{x=x_0,y=y_0}(x-x_0)^2 \\ &\quad + \left.\frac{\partial f}{\partial x}\frac{\partial f}{\partial y}\right|_{x=x_0,y=y_0}(x-x_0)^2 \\ &\quad + \frac{1}{2!}\left.\frac{\partial^2 f}{\partial x^2}\right|_{x=x_0,y=y_0}(x-x_0)^2 \end{aligned} \tag{2.16}$$

There are neater ways to write this once we have matrix formalism under our belt.

Chapter 3

Ordinary Differential Equations

This chapter is about "ordinary" differential equations, that is, equations whose solutions are functions of a single independent variable. We will cover "partial" differential equations in Section 4.5.

Remember that this course is about mathematics as applied to problems in physics. There are many subtleties in the mathematics of differential equations that will gloss over or outright ignore. For this reason, I encourage all physics students to take a mathematics course in differential equations. Temple's Mathematics Department offers the course MATH 2045 *Differential Equations with Linear Algebra*, which I believe to be a good option.

An excellent textbook is *Elementary Differential Equations and Boundary Value Problems*, by Boyce, DiPrima, and Meade, now in its 11th edition, published by Wiley. The ISBN is 978-1-119-32063-0. It's the book I learned the subject from (in its 2nd edition) and updates over the years have kept up with education research and the greater available of computing capability for numerical solutions.

3.1 Differential Equations and their Solutions

Differential equations are equations that involve derivatives of some function. A solution to a differential equation is the function itself. For each order of derivative in the differential equation, you have to specify some "boundary condition" to go along with all of the lower order derivatives and for the function. (In physics, when the differential equation involves functions of, and derivatives with respect to, time, we call the boundary conditions "initial conditions.") Sometimes you will have a set of differential equations involving different functions, that can appear in some or all of the equations. This is called a system of "coupled" differential equations.

It's worth pointing out at the start that Physics is generally formulated in terms of differential equations. Newton's Second Law $\vec{F} = m\vec{a}$, Maxwell's Equations, and the Schrödinger Equation are all differential equations. Einstein's gravitational field equations, too.

There are very many techniques for solving the very many different types of differential equations. We'll see a small number of these techniques in this course, but it is often the case that you can just use your wits to figure out a solution. As with most things, practice makes perfect.

In broad terms, there are two general classes of differential equations, called *Ordinary Differential Equations* (ODE's) and Partial Differential Equations (PDE's). An ODE has only one independent variable, which we will usually (but not always!) call x or t, and the derivatives of the solution function will only be ordinary derivatives with respect to this variable. The solution to a PDE will be a function of two or more variables, with various partial derivatives with respect to them.

The techniques for dealing with ODE's are very different than those for working with PDE's, so we discuss them separately. We take up a discussion of PDE's n Section 4.5.

3.1.1 Ordinary Differential Equations

An ordinary differential equation for a function $y = y(x)$ is an equation of the form

$$\frac{d^{(n)}y}{dx} = f\left(x, y, \frac{dy}{dx}, \frac{d^2y}{dx^2}, \cdots, \frac{d^{(n-1)}y}{dx^{n-1}}\right) \tag{3.1a}$$

where f is some function, and $d^{(n)}y/dx^n$ is the nth derivative of $y(x)$. We will often use the notation $y^{(n)}(x) = d^{(n)}y/dx^n$. Any solution to (3.1a) must also solve some given boundary conditions at a point $x = x_0$, namely

$$y(x_0) = y_0, \qquad y'(x_0) = y_0', \qquad y''(x_0) = y_0'', \ldots, \qquad y^{(n-1)}(x_0) = y_0^{(n-1)} \tag{3.1b}$$

If instead of x we use t (time) for the independent variable, then we refer to "initial conditions" instead of boundary conditions.

We call n the "order" of the differential equation, that is, the highest derivative that appears. An ODE of order n needs to have n boundary conditions. You can think of each of these conditions leading to determine the constant of integration that we'll get from integrating the derivatives.

If (3.1a) can be cast into the form

$$a_0(x)y + a_1(x)y' + a_2(x)y'' + \cdots + a_n(x)y^{(n)} = g(x) \tag{3.2}$$

then we call the differential equation "linear." If the function $g(x) = 0$ we call the equation "homogeneous." There are some general approaches we can take for linear, homogeneous equations, and these can be directly applied to linear inhomogeneous equations. Let's see how this works in general now. We will return to this in many examples later.

All linear, homogeneous differential equations have an extremely important property that is inherent in so many physical situations. This is the *principle of superposition* which says that

any linear combination of two solutions is also a solution. Writing $y(x) = c_1 y_1(x) + c_2 y_2(x)$, where $y_1(x)$ and $y_2(x)$ are both solutions to (3.2) and c_1 and c_2 are constants, then it is a simple matter to show that $y(x)$ is also a solution. For an nth order equation, we can expect to find n different *linearly independent* solutions so that

$$y(x) = c_1 y_1(x) + c_2 y_2(x) + \cdots + c_n y_n(x) \tag{3.3}$$

is the general solution. In principle, we can determine the constants c_1, c_2,..., c_n by applying the boundary conditions.

How do we know that the solutions $y_i(x)$ are linearly independent? There is a straightforward way to answer this using matrix manipulations.[1] We apply this solution to the boundary conditions and get a set of equations that can be written as

$$\begin{bmatrix} y_1(x_0) & y_2(x_0) & \cdots & y_n(x_0) \\ y_1'(x_0) & y_2'(x_0) & \cdots & y_n'(x_0) \\ \vdots & \vdots & \cdots & \vdots \\ y_1^{(n)}(x_0) & y_2^{(n)}(x_0) & \cdots & y_n^{(n)}(x_0) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} y_0 \\ y_0' \\ \vdots \\ y_0^{(n)} \end{bmatrix} \tag{3.4}$$

This set of equations only has a solution if the determinant of the matrix is nonzero, and this is the condition we need for the set of equations $y_i(x)$ to be linearly independent. This determinant is called the *Wronskian* and we write

$$W(x) = \begin{vmatrix} y_1(x) & y_2(x) & \cdots & y_n(x) \\ y_1'(x) & y_2'(x) & \cdots & y_n'(x) \\ \vdots & \vdots & \cdots & \vdots \\ y_1^{(n)}(x) & y_2^{(n)}(x) & \cdots & y_n^{(n)}(x) \end{vmatrix} \tag{3.5}$$

So, linear independence at a point $x = x_0$ requires that we have $W(x_0) \neq 0$. In most of the cases you'll see in physics, $W(x)$ will be nonzero for the entire relevant range of the independent variable x.

This is all fine for homogeneous linear equations, but what if the equation is inhomogeneous? In this case, your first job is to fine a "particular" solution $y_P(x)$ which solves (3.2) for nonzero $g(x)$. This solution does not need to have any constants that fit the boundary conditions, because once you have $y_P(x)$, you can add to it any solution (3.3) to the homogeneous equation and the result still solves (3.2). You then apply the boundary conditions to determine the constants c_i.

Again, we will see examples of all this in this chapter.

Finally, we point out that a nonlinear differential equation can also be homogeneous, but in this case you would have to cast it into a form using a change of variables so that it has no

[1] We won't be discussing matrices until Chapter 6, so if you're unfamiliar with this, just skip over this discussion. I'll be illustrating with examples later in this chapter.

remaining explicit function of x with no factor that depends on y or its derivatives. For a first order equation, for example, a homogenous differential equation is one of the form

$$\frac{dy}{dx} = G\left(\frac{y}{x}\right)$$

I don't think you'll ever have occasion in your upper level physics courses to deal with inhomogeneous nonlinear differential equations.

3.1.2 Existence and Uniqueness

It might bother you that I have just gone ahead willy nilly writing down some properties of differential equations and implying that I can find solutions with these ideas. But maybe there are other solutions to the equation and boundary conditions that can't be found by following these properties? Or maybe there is no solution to the equation after all?

In fact, the answer is "No" to both questions. For all of the cases we'll study in this course, any given ODE or PDE, along with a set of boundary conditions, has exactly one solution. That is, the solution *exists* and is *unique*. I'm not going to prove this, but you'll do so in a real course in differential equations, and see the conditions that need to be satisfied for the proof.

Nevertheless, this is a very powerful statement. We can go ahead and find a solution to a differential equation, and the boundary conditions, any way that we want, and be assured that it is the right answer. My favorite example of this is the "image charge" approach to solving boundary value problems in electrostatics, something you'll encounter in your Electricity & Magnetism course.

3.1.3 Using scaled variables

We have already learned about dimensional analysis. This will allow you to identify fixed quantities in your differential equation that have dimensions of, say, distance, time, energy,..., and then define new variables that are dimensionless.

If your problem is one that requires you to make approximations as to whether something is "big" or "small", then scaling the variables lets you decide this based on whether something is much larger or much smaller than unity. Also, if your problem is suited to solving numerically with MATHEMATICA or some other application, then it will be very handy to express your independent and dependent variables in dimensionless form by dividing them by some appropriate scale.

We'll see lots of examples of this, but here's a simple one. The differential equation for the simple harmonic oscillator in one dimension $x(t)$, from $F = ma$ written as $ma - F = 0$, is

$$m\frac{d^2x}{dt^2} + kx = 0$$

The frequency scale is $\omega = (k/m)^{1/2}$. (You should confirm for yourself that this has dimensions of inverse time!) Defining a dimensionless time $\tau = \omega t$ turns the equation into

$$\frac{d^2x}{d\tau^2} + x = 0$$

and now you have a natural way to discuss the oscillator in terms of short times, i.e. $\tau \ll 1$, or long times, i.e. $\tau \gg 1$. (This is actually more useful when the oscillator is also subjected to a damping force and and oscillating forcing function, each of which introduce their own time scales.)

3.2 First Order Equations

First we'll make some general comments and observations about first order equations, and then do a couple of examples. Remember, though, that sometimes the best way to solve the equation is to look at it and see your way through without having to go to a menu of techniques!

If a differential equation has the form

$$\frac{dy}{dx} = \frac{p(x)}{q(y)} \qquad \text{i.e.} \qquad q(y)dy = p(x)dx$$

then it is called *separable*. If the antiderivatives $Q(y)$ and $P(x)$ are known, then just integrate both sides to get

$$Q(y) = P(x) + C$$

where the constant of integration C is determined from the boundary condition.

Next consider an equation of the form

$$P(x,y)dx + Q(x,y)dy = 0$$

If it happens to be that

$$\frac{\partial P}{\partial y} = \frac{\partial Q}{\partial x}$$

then we call the differential equation *exact* because there would be a function $\psi(x,y)$ such that

$$\frac{\partial \psi}{\partial x} = P(x,y) \qquad \text{and} \qquad \frac{\partial \psi}{\partial y} = Q(x,y)$$

and the equation can be written as an exact differential and integrated trivially. If the equation is not exact, then sometimes you can multiply through by a factor $\mu(x)$ that renders the equation exact. The function $\mu(x)$ is called an "integrating factor."

The use of integrating factors can be demonstrated explicitly for the inhomogeneous linear first order equation

$$\frac{dy}{dx} + p(x)y = g(x) \tag{3.6}$$

If you define the integrating factor as the exponential of the antiderivative of $p(x)$,

$$\mu(x) = \exp\left[\int p(x)dx\right]$$

and multiply through by $\mu(x)$, then it is fairly obvious that

$$\frac{d}{dx}\left[\mu(x)y(x)\right] = \mu(x)g(x)$$

and so the general solution is

$$y(x) = \frac{1}{\mu(x)}\left[\int \mu(x)g(x)\,dx + C\right]$$

where, once again, we determine C from whatever is the boundary condition.

3.2.1 Example: Radioactive Decay

Quantum mechanics predicts that the probability of radioactive decay for an unstable nucleus to decay in any given short time period dt is λdt, where λ is a constant that can be calculated, in principle, from the properties of the nucleus. Suppose that you start with a given number N_0 of nuclei. Then you expect the number $N(t)$ to decrease over time because they decay. Given the probability λdt, the change in the number of nuclei during this time period is $dN = -\lambda N\,dt$.

This all leads to the differential equation and initial condition

$$\frac{dN}{dt} = -\lambda N(t) \qquad N(0) = N_0$$

The form of this equation makes it simple to guess the answer. With the derivative proportional to the function, you know that the solution has to be some exponential. Let's use a technique from Section 3.2 to get the solution, though.

This is a perfect example of a separable equation. We write

$$\frac{dN}{N} = -\lambda\,dt \qquad \text{so} \qquad \int\frac{dN}{N} = -\lambda\int dt \qquad \text{or} \qquad \log N = -\lambda t + C$$

Exponentiating both sides give us $N = e^{-\lambda t}e^{C}$. Applying the boundary condition gives $N_0 = e^{C}$. Therefore, the solution is

$$N(t) = N_0 e^{-\lambda t}$$

Typically, we tabulate the *half-life* $t_{1/2}$ of radioactive nuclei, namely the time it takes for the sample to decay to one half its value. That is

$$\frac{1}{2} = e^{-\lambda t_{1/2}} \qquad \text{so} \qquad t_{1/2} = \frac{1}{\lambda}\log 2$$

This law also governs the decay of elementary particles and excited atomic states. For some bizarre historical reason, however, we do not quote the half-life for these decays. Instead, we use the mean life $\tau \equiv 1/\lambda$.

3.2.2 Example: Falling under drag

This is a simple problem that is intuitively easy to visualize, and is a problem that can be solved using either separability or with an integrating factor.

A mass m falls vertically, starting from rest at height h. In addition to gravity (near the Earth's surface) there is a drag force proportional to the velocity. Find the velocity as a function of time. Then find the vertical position as a function of time. (This involves writing down and solving a first order equation, and then another first order equation.)

Let $v(t)$ be the velocity and $y(t)$ be the vertical position as a function of time. Write the drag force as $-bv$ where $b > 0$. (The sign ensures that the drag force is opposite to the direction of velocity.) Assume that positive v is "up." Then

$$m\frac{dv}{dt} = -mg - bv \qquad \text{so} \qquad \frac{dv}{dt} + \frac{b}{m}v = -g$$

which is exactly the form given by (3.6). So, let's approach the solution using an integrating factor. We have

$$\mu(t) = \exp\left[\int \frac{b}{m}\,dt\right] = e^{bt/m}$$

The solution is then

$$v(t) = \frac{1}{e^{bt/m}}\left[\int e^{bt/m}(-g)\,dt + C\right] = e^{-bt/m}\left[-\frac{mg}{b}e^{bt/m} + C\right] = -\frac{mg}{b}\left[1 - \frac{b}{mg}Ce^{-bt/m}\right]$$

The initial condition is $v(0) = 0$ so $C = mg/b$ and we finally have

$$v(t) = -\frac{mg}{b}\left[1 - e^{-bt/m}\right]$$

It is always important to check that the result makes sense. Firstly, $v(0) = 0$, as we required. Secondly, $v(t) < 0$ for $t > 0$, which is also correct, since the mass falls from rest. Thirdly, as you might have expected, a "terminal velocity" $v_{\text{term}} = mg/b$ is reached for long times. You expect this because if the mass is moving fast enough, then the force of gravity mg is exactly balanced by the drag force bv.

We can also do some simple dimensional analysis to check the result. For example, for the exponential argument to make sense, the quantity b/m must have the dimensions of inverse time. Since bv is a force, we must have

$$[b][v] = [b]LT^{-1} = MLT^{-2} \qquad \text{so} \qquad [b] = MT^{-1}$$

and, indeed, b/m has dimensions of inverse time.

Now, in this case, the result for $v(t) = dy/dt$ can easily be integrated to find $y(t)$ subject to the initial condition $y(0) = h$. This gives the position as a function of time. This is a cheaters way of solving the second order equation for $y(t)$, and that's fine, but not always an option.

Finally, note that we could also have approached this as a separable equation. We have

$$\frac{dv}{1+bv/mg} = -g\,dt \qquad \text{so} \qquad \int_0^v \frac{dv}{1+bv/mg} = -g\int_0^t dt$$

where we integrate both sides, the left from 0 to v and the right from 0 to t. (We can change the integration variables to "primes" if that makes people feel better, but you want to get used to not having to do that.) Then

$$\frac{mg}{b}\log\left(1+\frac{b}{mg}v\right) = -gt \qquad \text{so} \qquad v(t) = -\frac{mg}{b}\left(1-e^{-bt/m}\right)$$

3.2.3 Example: The rocket equation

Mention the conservation of momentum, namely $dp/dt = 0$ if no external forces act on an object with mass m and velocity v, with $p = mv$. Now imagine a rocket, burning fuel and therefore decreasing its mass while increasing its velocity. If $v_{\rm ex}$ is the exhaust velocity, relative to the rocket, the momentum of the rocket plus the ejected fuel at a time $t + dt$ is

$$p(t+dt) = (m+dm)(v+dv) - dm(v-v_{\rm ex}) = mv + mdv + v_{\rm ex}dm$$

Note that I neglected the second order term $(dm)(dv)$. Now the change in momentum is

$$dp = p(t+dt) - mv = mdv + v_{\rm ex}dm = 0$$

which is a separable first order differential equation. We can write

$$v_{\rm ex}\frac{dm}{m} = -dv \qquad \text{so} \qquad v_{\rm ex}\log\frac{m}{m_0} = -v + v_0$$

where $v = v_0$ is the initial velocity and $n = m_0$ is the initial mass. It is probably handier to write this as $v = v_0 + v_{\rm ex}\log(m_0/m)$. See Taylor *Classical Mechanics* for more discussion.

3.3 Second Order Linear Equations

Given Newton's Second Law, written as $m\ddot{x}(t) = F(x,t)$, it is clear that second order ordinary differential equations are ubiquitous in Physics. In this section we will focus on linear differential equations. Of course, the form of the force $F(x,t)$ can lead to nonlinear equations and various associated (and fascinating) physical phenomena. More often than not, however, these equations need to be solved numerically, so we leave them to the laboratory portion of this course.[2]

[2]Chapter 12 of *Classical Mechanics* by Taylor has a terrific presentation of nonlinear systems and chaos using the forced, damped pendulum. Numerical calculations are carried out using MATHEMATICA.

You should realize that in case where the function is explicitly "missing" in (3.1a), that is

$$\frac{d^2y}{dx^2} = f\left(x, \frac{dy}{dx}\right)$$

we can reduce the problem to a first order equation by writing $v(x) \equiv y'(x)$ and then solving for $v(x)$. This is one of the approaches we used in Section 3.2.2. It is not always an easy matter, though, to integrate the equation for $v(x)$ in order to get $y(x)$.

Now we focus on linear second order equations. Following (3.1a), we are now working with the functional form

$$f\left(t, y, \frac{dy}{dx}\right) = g(x) - p(x)\frac{dy}{dx} - q(x)y$$

we are working with differential equations of the form

$$y'' + p(x)y' + q(x)y = g(x)$$

to be solved for the function $y(x)$ with the boundary conditions $y(x_0) = y_0$ and $y'(x_0) = y_0'$. We will use the machinery outlined in Section 3.1.1 and go through some examples. Remember in particular that, for a linear inhomogeneous equation, we can solve the homogeneous equation after finding a particular solution to the inhomogeneous equation, and use this combination to find the coefficients c_i that satisfy the boundary conditions.

3.3.1 Constant Coefficients

Before moving on to physical examples, let's work on what is likely the simplest example of a second order linear differential equation, namely one that is homogeneous with constant coefficients. That is, an equation of the form

$$ay'' + by' + cy = 0$$

where a, b, and c are real constants. Relying on existence and uniqueness, let's try a solution that looks like an exponential, but with some freedom that we can exploit. We can make the "ansatz" (i.e. "guess") that the solution is of the form $y(x) = e^{\alpha x}$ where α is yet to be determined. Substituting into our differential equation gives

$$\alpha^2 a e^{\alpha t} + \alpha b e^{\alpha t} + c e^{\alpha t} = 0$$

Canceling out the factor $e^{\alpha t}$ leaves us with the quadratic equation for α

$$a\alpha^2 + b\alpha + c = 0$$

known as the "characteristic equation." It has the solution

$$\alpha = -\frac{b}{2a} \pm \frac{\sqrt{b^2 - 4ac}}{2a} \equiv \alpha_{1,2}$$

Consequently, we expect that we have two linearly independent solutions

$$y_1(x) = e^{\alpha_1 x} \qquad \text{and} \qquad y_2(x) = e^{\alpha_2 x}$$

If it turns out that $b^2 - 4ac < 0$, then α_1 and α_2 will be complex, and Euler's Formula will give us sines and cosines. Recall Section 2.4.3.

A complication arises if $b^2 - 4ac = 0$. In this case, there is only one linearly independent solution given the $e^{\alpha t}$ ansatz. We have to figure out some other way to get a second solution. Then, of course, if we want to solve an inhomogeneous equation, we need to find a particular solution.

Let's illustrate all this with some specific examples. First, consider the homogeneous equation

$$y'' - y = 0 \qquad \text{with} \qquad y(0) = 2 \qquad \text{and} \qquad y'(0) = -1$$

That is, $a = 1$, $b = 0$, and $c = -1$, giving $\alpha = \pm 1$. That is, $\alpha = \pm 1$, in which case $y_1(x) = e^x$ and $y_2(x) = e^{-x}$ so that

$$y(x) = c_1 y_1(x) + c_2 y_2(x) = c_1 e^x + c_2 e^{-x}$$

The boundary conditions tell us that $2 = c_1 + c_2$ and $-1 = c_1 - c_2$ so that $c_1 = 1/2$ and $c_2 = 3/2$. Thus, the complete solution is

$$y(x) = \frac{1}{2} e^x + \frac{3}{2} e^{-x}$$

It is worthwhile to check the Wronskian to see that the two solutions are indeed linearly independent. Following (3.5) we write

$$W(x) = \begin{vmatrix} y_1(x) & y_2(x) \\ y_1'(x) & y_2'(x) \end{vmatrix} = \begin{vmatrix} e^x & e^{-x} \\ e^x & -e^{-x} \end{vmatrix} = -2$$

which of course is nonzero for all x. The two solutions $y_1(x)$ and $y_2(x)$ are linearly independent for all $x \in \mathbb{R}$.

Next consider the similar but inhomogeneous equation

$$y'' - y = 1 \qquad \text{with} \qquad y(0) = 2 \qquad \text{and} \qquad y'(0) = -1$$

with the same boundary conditions. It is simple to guess the particular solution $y_P(x) = 1$. Therefore, the general solution is

$$y(x) = y_P(x) + c_1 y_1(x) + c_2 y_2(x) = 1 + c_1 e^x + c_2 e^{-x}$$

and the boundary conditions tell us that $2 = 1 + c_1 + c_2$ and $-1 = c_1 - c_2$ so that $c_1 = 0$ and $c_2 = 1$, giving us the complete solution

$$y(x) = 1 + e^{-x}$$

You should check that this satisfies the differential equation as well as the boundary conditions.

Now let's try a third and final example. Consider the equation

$$y'' + 4y' + 4y = 0$$

for which the characteristic equation becomes $\alpha^2 + 4\alpha + 4 = (\alpha + 2)^2 = 0$. There is only one solution, namely $\alpha = -2$. How can we find the second linearly independent solution so that we can satisfy arbitrary boundary conditions?

Once again, we are rescued thanks to existence and uniqueness. Let's guess that if we modify our one solution by a function $v(x)$, that is $y_2(x) = v(x)e^{-2x}$, and substitute it into our differential equation, then we should be able to find a differential equation for $v(x)$ that we can solve. Doing the work,

$$\begin{aligned}
y_2(x) &= v(x)e^{-2x} \\
y_2'(x) &= v'(x)e^{-2x} - 2v(x)e^{-2x} \\
y_2''(x) &= v''(x)e^{-2x} - 2v'(x)e^{-2x} - 2v'(x)e^{-2x} + 4v(x)e^{-2x} \\
&= v''(x)e^{-2x} - 4v'(x)e^{-2x} + 4v(x)e^{-2x} \\
y_2'' + 4y_2' + 4y_2 &= v''(x)e^{-2x} - 4v'(x)e^{-2x} + 4v(x)e^{-2x} \\
&\quad +4v'(x)e^{-2x} - 8v(x)e^{-2x} + v(x)e^{-2x} \\
&= v''(x)e^{-2x} = 0
\end{aligned}$$

Aha! We want a function $v(x)$ that satisfies $v''(x) = 0$. Obviously, that is $v(x) = c_1 + c_2 x$, and the general solution to this homogenous second order homogeneous equation is

$$y(x) = (c_1 + c_2 x)e^{-2x}$$

We don't have to bother with considering $y_1(x)$ from above, because this approach alone gave us a general solution with two constants. Existence and uniqueness tell us that we are done.

3.4 Harmonic Motion in One Dimension

Let's now use this machinery to study harmonic motion, a subject we started in Section 2.4.3. You likely saw this in some detail in detail in Wave Physics, so I'll treat this as a review. It is a very useful example because, in addition to being very important physically, it embodies so much of the mathematics we have discussed to this point, as well as mathematics we have yet to get to.

3.4.1 Simple harmonic motion

The motion of a mass m subject to a linear restoring force $-kx$, with no other forces in the direction of motion, is called *Simple Harmonic Motion*. This problem was worked out

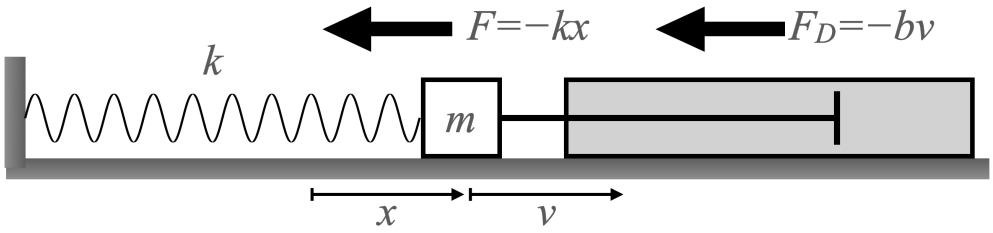


Figure 3.1: The physical situation leading to damped harmonic oscillation. In addition to the restoring force $F = -kx$, there is also a linear damping force $F_D = -bv$ which acts in the direction opposite of the velocity.

thoroughly in Section 2.4.3, but let's take a moment to couch that discussion in the language of second order linear differential equations.

We solved the differential equation (2.11), which we rewrite as

$$x''(t) + \omega_0^2 x(t) = 0 \qquad x(0) = x_0 \qquad x'(0) = v_0$$

where I have included the initial conditions. This is an example of a second order linear ODE with constant coefficients, which we discussed in detail in Section 3.3.1. We approached the solution in a couple of ways, one of which was to use the ansatz $x(t) = e^{\alpha t}$. In this case, the characteristic equation is

$$\alpha^2 + \omega_0^2 \qquad \text{so} \qquad \alpha = \pm i\omega_0$$

in which case the general solution is

$$x(t) = c_1 e^{i\omega_0 t} + c_2 e^{-i\omega_0 t}$$

Applying the initial conditions led us to the complete solution (2.15), that is

$$x(t) = R\cos(\omega_0 + \phi)$$

where (2.14) gives R and ϕ in terms of x_0 and v_0.

Recall also that we used Simple Harmonic Motion as an example of writing a differential equation in terms of scaled variables. See Section 3.1.3.

3.4.2 Damped harmonic motion

Now let's take the next step and add a (linear) damping force to the mass. See Figure 3.1. Newton's Second Law now says that

$$m\frac{d^2x}{dt^2} = -kx - bv = -kx - b\frac{dx}{dt}$$

If we define $\beta \equiv b/2m$, and keep our definition $\omega_0^2 = k/m$, then the differential equation we need to solve is

$$x''(t) + 2\beta x'(t) + \omega_0^2 x(t) = 0 \tag{3.7}$$

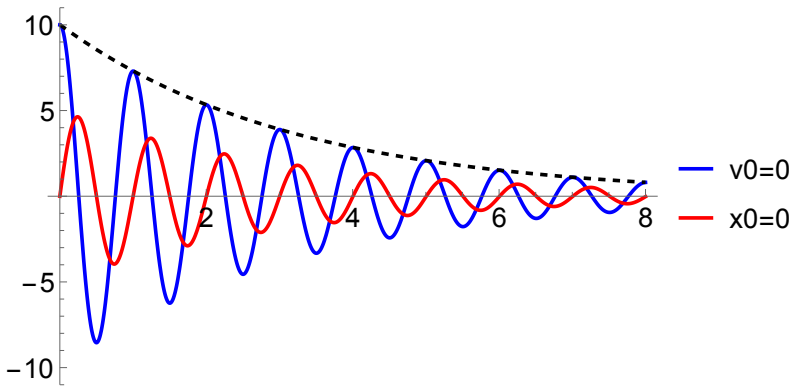


Figure 3.2: Example of under damped harmonic oscillations. The curves are drawn for $\omega_0 = 2\pi$ and $\beta = 0.05\omega_0$. The curve labeled $v_0 = 0$ uses $x_0 = 10$, and the curve labeled $x_0 = 0$ uses $v_0 = 5\omega_0$. The dashed line shows the envelope of the decreasing exponential amplitude, that is $Re^{-\beta t}$ with the notation from the text.

Once again, this is a linear second order homogeneous differential equation with constant coefficients. Applying our ansatz $x(t) = e^{\alpha t}$ gives the characteristic equation

$$\alpha^2 + 2\beta\alpha + \omega_0^2 = 0 \qquad \text{so} \qquad \alpha = -\beta \pm \sqrt{\beta^2 - \omega_0^2}$$

In the familiar case known as *under damping*, $\beta < \omega_0$ and the argument of the square root is negative. Therefore α is complex and we write $\alpha = -\beta \pm i\omega_1$ where $\omega_1 = \sqrt{\omega_0^2 - \beta^2}$ and the general solution takes the form

$$x(t) = e^{-\beta t}\left(c_1 e^{i\omega_1 t} + c_2 e^{-i\omega_1 t}\right) = Re^{-\beta t}\cos(\omega_1 t + \phi) \tag{3.8}$$

where the constants c_1 and c_2, or R and ϕ, are determined from the initial conditions. Figure 3.2 plots two examples of damped oscillatory motion.

A useful quantity when discussing damped oscillations, especially for very weakly damped oscillations for which $\beta \ll \omega_0$, is the Q (for "Quality") factor, defined as

$$Q = \frac{\omega_0}{2\beta} \tag{3.9}$$

This quantity is best interpreted in terms of the energy of the oscillator. When the mass is at its maximum position, that is the amplitude, all of the oscillator's energy is in potential energy which is proportional to the square of the amplitude. The amplitude in (3.8) decreases like $e^{-\beta t}$, so the energy of the oscillator depends on time as $E(t) = E(0)e^{-2\beta t}$. Therefore, for the weakly damped case, the change in the energy over one period of oscillation is

$$\Delta E = E(t) - E\left(t + \frac{2\pi}{\omega 0}\right) = E(t)\left[1 - e^{-2\beta(2\pi/\omega_0)}\right] \approx E(t)\,2\pi\,\frac{2\beta}{\omega_0} \qquad \text{for} \qquad \beta \ll \omega_0$$

In other words, for a weakly damped oscillator, the fractional change in energy over one cycle is $\Delta E/E = 2\pi/Q$. A large value of Q means that the oscillator is not very "lossy",

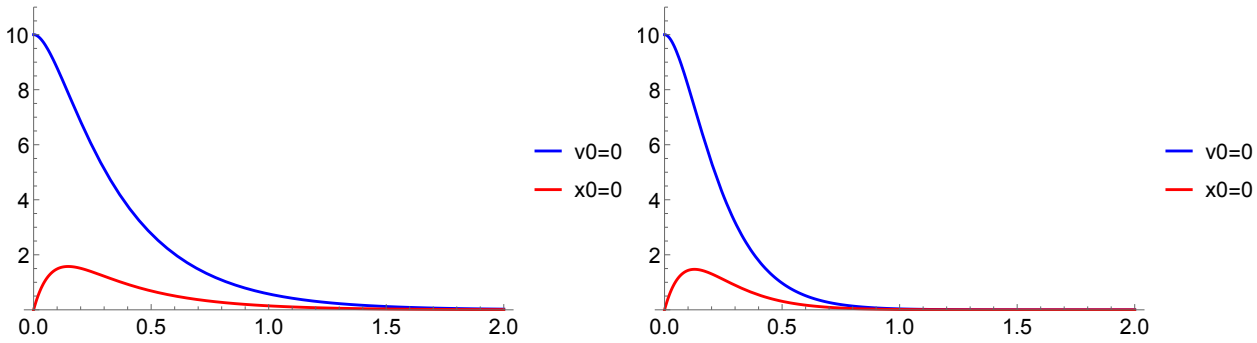


Figure 3.3: Examples of under damped (left) and critically damped (right) motion. The same initial conditions were used as those in Figure 3.2, and once again $\omega_0 = 2\pi$. The under damped case uses the value $\beta = 1.25\omega_0$. Notice that the critically damped case approaches zero more rapidly.

and therefore of a higher "quality." We will return to the usefulness of Q when we study forced, damped oscillations in Section 3.4.3.

As discussed in Section 3.3.1, the solution for the *over damped* case when $\beta > \omega_0$ is

$$x(t) = c_1 e^{\alpha_1 t} + c_2 e^{\alpha_2 t} \qquad \alpha_{1,2} = -\beta \pm \sqrt{\beta^2 - \omega_0^2}$$

and the *critically damped* case for $\beta = \omega_0$ has the solution

$$x(t) = (c_1 + c_2 t)e^{-\beta t}$$

Figure 3.3 plots these solutions for the same initial conditions as in Figure 3.2. Of course, the solutions do not oscillate in either of these cases, and the critically damped solution approaches zero most rapidly.

3.4.3 Forced damped harmonic motion

Now imagine what happens if we "force" the oscillator by driving the equilibrium point back and forth in an oscillatory manner whose frequency we can control. See Figure 3.4. The other side of the spring from the mass is no longer fixed, but driven along a point $x_0 = B\cos\omega t$. This means that the force from the spring on the mass is $F = -k(x - x_0)$ and the differential equation that describes the system is given by

$$mx''(t) + bx'(t) + kx(t) = kx_0 = kB\cos\omega t$$

Defining $\beta = b/2m$ and $\omega_0^2 = k/m$ as before, and also defining $\gamma = kB/m$, we have

$$x''(t) + 2\beta x'(t) + \omega_0^2 x(t) = \gamma\cos\omega t \tag{3.10}$$

This is a linear, second order, inhomogeneous differential equation with constant coefficients, a case that we also treated in Section 3.3.1.

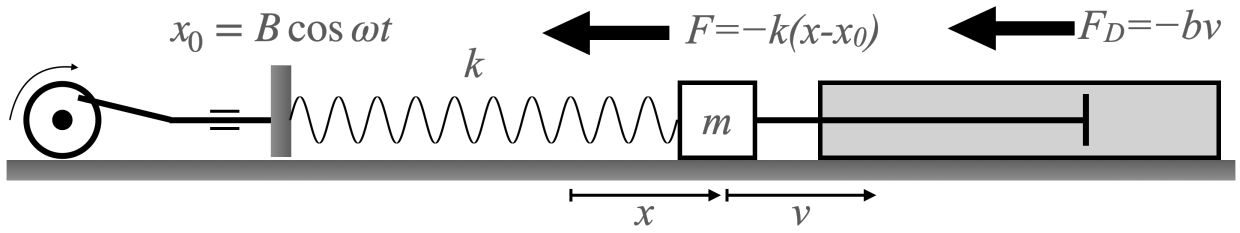


Figure 3.4: The physical situation leading to forced damped harmonic oscillation. The left side attachment point of the spring is no longer fixed, but instead is forced to oscillate sinusoidally by forcing it to move with angular frequency ω. This modifies the restoring force of the spring on the mass ot be $F = -k(x - x_0)$ where $x_0 = B\cos\omega t$.

The only tricky part to solving this problem is to find a particular solution. Having that, we just need to add it to the general solution for the homogeneous equation, and then find the two constants by applying the initial conditions. Looking at (3.10), however, it is by no means obvious what is the particular solution. On the other hand, it is probably some linear combination of $\cos\omega t$ and $\sin\omega t$ so we write

$$x_P(t) = a\cos\omega t + b\sin\omega t$$

and insist that this form solve (3.10) in order to determine a and b.[3] We find

$$-a\omega^2\cos\omega t - b\omega^2\sin\omega t - 2\beta a\omega\sin\omega t + 2\beta b\omega\cos\omega t + \omega_0^2 a\cos\omega t + \omega_0^2 b\sin\omega t = \gamma\cos\omega t$$

Gathering up terms proportional to $\cos\omega t$ and $\sin\omega t$ give us the equations

$$\begin{aligned}(\omega_0^2 - \omega^2)a + 2\beta\omega b &= \gamma \\ -2\beta\omega a + (\omega_0^2 - \omega^2)b &= 0\end{aligned}$$

Solving this pair of equations for a and b is straightforward, albeit tedious. (Or you can do what I did and ask MATHEMATICA to solve them for you.) You find

$$a = \frac{\gamma\,(\omega_0^2 - \omega^2)}{4\beta^2\omega^2 + (\omega_0^2 - \omega^2)^2} \qquad \text{and} \qquad b = \frac{2\beta\gamma\omega}{4\beta^2\omega^2 + (\omega_0^2 - \omega^2)^2}$$

It makes sense to write

$$A(\omega) = \sqrt{a^2 + b^2} = \frac{\gamma}{\sqrt{4\beta^2\omega^2 + (\omega_0^2 - \omega^2)^2}} \tag{3.11a}$$

$$\text{and} \qquad \tan\Phi(\omega) = \frac{b}{a} = \frac{2\beta\omega}{\omega_0^2 - \omega^2} \tag{3.11b}$$

[3] A much slicker way to do this is to let $x(t)$ be complex, and write the right side of the equation as $\gamma e^{i\omega t}$. I'm going to take the more straightforward approach here.

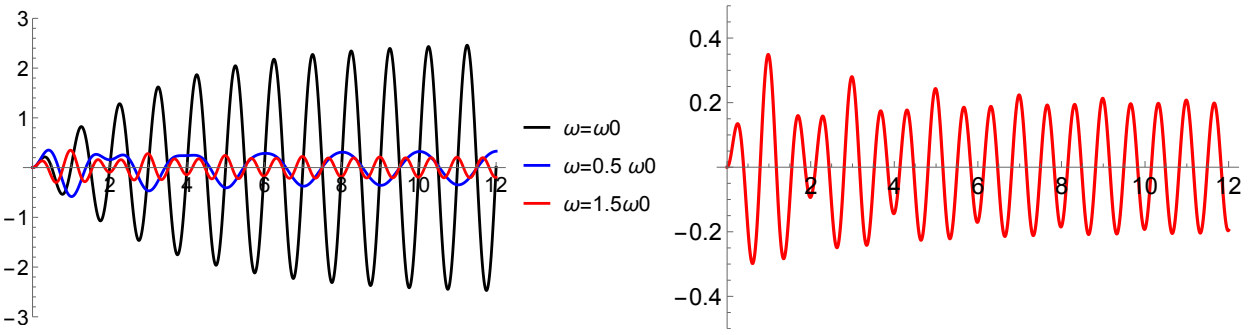


Figure 3.5: Plot of the motion $x(t)$ of an underdamped oscillator driven at three different frequencies ω relative to the natural frequency ω_0. The plot assumes $\omega_0 = 2\pi$, $\beta = 0.05\omega_0$ and uses initial conditions $x(0) = 0$ and $x'(0) = 0$. The driving amplitude is $\gamma = 10$. The plot on the right is an expanded view of the $\omega = 1.5\omega_0$ curve on the left.

in which case we have

$$x_P(t) = A\cos\Phi\cos\omega t + A\sin\Phi\sin\omega t = A\cos(\omega t - \Phi)$$

Now we can use the results of Section 3.4.2 to write the complete solution to (3.10) as

$$x(t) = c_1 e^{\alpha_1 t} + c_2 e^{\alpha_2 t} + A\cos(\omega t - \Phi)$$

where $\alpha_1 = -\beta + \sqrt{\beta^2 - \omega_0^2}$ and $\alpha_2 = -\beta - \sqrt{\beta^2 - \omega_0^2}$ are complex for the oscillating (under damped) case ($\beta < \omega_0$) or real for the over damped case ($\beta > \omega_0$), and

$$x(t) = (c_1 + c_2 t)e^{-\beta t} + A\cos(\omega t - \Phi)$$

for the critically damped case ($\beta = \omega_0$). For all cases, we find c_1 and c_2 by applying initial conditions $x(0) = x_0$ and $x'(0) = v_0$.

Figure 3.5 shows the motion of an oscillator that starts from rest at $x = 0$, but is set in motion by the driving force. The motion is plotted for three different driving frequencies. The amplitude is much larger for $\omega = \omega_0$ than for the other two choices. This is not unexpected, given the denominator in our expression for $A(\omega)$.

The figure also includes an expanded view of the motion for $\omega = 1.5\omega_0$. Notice how the motion appears somewhat irregular for the first several periods before settling into a steady motion at the driving frequency. This is the effect of the *transients* that are the elements of the homogeneous solution. The transients die away with a time constant $1/\beta$.

The large amplitude in Figure 3.5 when $\omega \approx \omega_0$ is the familiar phenomenon known as *resonance*. When you drive any underdamped oscillator at a frequency close to its natural frequency, it responds with a large amplitude. Figure 3.6 shows explicitly how the amplitude depends on the driving frequency, showing a "resonance peak." Note also that the relative phase between the response and the driving signal varies with frequency as well. For low

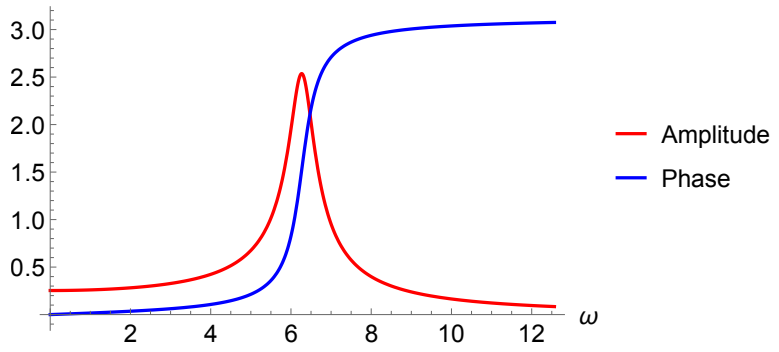


Figure 3.6: The amplitude $A(\omega)$ and phase $\Phi(\omega)$ for the particular solution $x_P(t)$, using the same parameters as in Figure 3.5. The peak in the amplitude is for ω near ω_0, which is where the phase Φ rises through 90°.

frequencies, the mass responds directly in phase with the driver, while for frequencies rather larger than the natural frequency, the response is 180° out of phase.

Resonance phenomena are ubiquitous in nature. The mathematics of an electrical oscillator made from a resistor, capacitor, and inductor obeys exactly the same differential equations that we have studied here. Quantum mechanical scattering is another well known system that displays resonance under the right conditions. There are also many examples in the response of living systems to oscillatory driving functions. In all cases, there is a peak in the amplitude, and a relative phase between the drive and response which rises from zero through 90° at resonance, and levels out to 180° out of phase at high frequencies.

Finally, consider the amplitude function $A(\omega)$ from (3.11a) for the weak damping situation $\beta \ll \omega_0$. The peak in the amplitude is near $\omega = \omega_0$ as see in Figure 3.6. We can also determine the "width" of the peak by calculating the values of ω for $A(\omega) = A_{\max}/\sqrt{2} \approx \gamma/2\sqrt{2}\beta\omega_0$. (We choose a fall by $\sqrt{2}$ because it is when the energy falls to one half its maximum value.) This occurs when

$$\sqrt{4\beta^2\omega^2 + (\omega_0^2 - \omega^2)^2} = 2\sqrt{2}\beta\omega_0$$

Substituting $\omega \approx \omega_0$ in the first term under the square root, we find $(\omega_0^2 - \omega^2)^2 = 4\beta^2\omega_0^2$. Solving for ω gives

$$\omega = \left[\omega_0^2 \pm 2\beta\omega_0\right]^{1/2} = \omega_0 \left[1 \pm \frac{2\beta}{\omega_0}\right]^{1/2} \approx \omega_0 \left[1 \pm \frac{\beta}{\omega_0}\right]$$

Therefore the fractional"width" of the resonance $\Delta\omega/\omega_0 = 2\beta/\omega_0 = 1/Q$, the "quality factor" from (3.9). This is a useful quantity for describing the performance of many resonant systems.

3.5 Series Solutions for Second Order Equations

So far, even though we've been talking about differential equations in general terms, the only solution we've come up with for linear second order ODE's is for the case where the homogeneous equation has constant coefficients. Indeed, there are many other examples of important second order linear ODE's in the physical sciences. Are there general approaches we can use to address them?

We learned in Chapter 2 that we can represent functions by infinite power series. We can take an approach, then, where the differential equation defines the function, and then we can use a power series to try and craft the solution. In fact, this approach works very well.

The basic idea is the following. Start with the homogeneous equation

$$r(x)y''(x) + p(x)y'(x) + q(x)y(x) = 0$$

and write the solution as a power series with unknown coefficients, that is

$$y(x) = a_0 + a_1 x + a_2 x^2 + \cdots = \sum_{n=0}^{\infty} a_n x^n$$

Substitute this form into the differential equation and manipulate the terms to find a "recursion relation" that relates a coefficient a_{n+2} to coefficients a_{n+1} and/or a_n. The coefficients a_0 and a_1 remain as the constants of integration, which get determined using the boundary conditions $y(0) = y_0$ and $y'(0) = y'_0$.

This approach works for a lot of problems, and we'll be discussing them soon. It doesn't always work, though. Remember that you have existence and uniqueness on your side, so variations of this approach can be used if necessary.

One variation is that the boundary values might be specified for $x \to \pm\infty$, a common situation in Quantum Mechanics. This variation tends to lead to the series being truncated, so the solution is actually a polynomial.

Another variation, known as the *Method of Frobenius*, is to write

$$y(x) = x^s \sum_{n=0}^{\infty} a_n x^n = \sum_{n=0}^{\infty} a_n x^{s+n}$$

and use the differential equation to constrain, or determine, the value of s.

3.5.1 Simple examples

Let's do some examples where we know what the answer has to be, and use these to illustrate how the series solution approach works. Nothing about the approach is restricted to second order equations, so let's start with

$$y'(x) = y(x)$$

Of course, the solution is $y(x) = ce^x$ where c is a constant. Inserting the series we have

$$\sum_{n=0}^{\infty} n a_n x^{n-1} = \sum_{n=0}^{\infty} a_n x^n \tag{3.12}$$

Now look at the sum on the left. The first term ($n = 0$) is manifestly zero, so we can start the sum from $n = 1$ and then switch to a dummy index $m = n - 1$. This gives

$$\sum_{n=0}^{\infty} n a_n x^{n-1} = \sum_{n=1}^{\infty} n a_n x^{n-1} = \sum_{m=0}^{\infty} (m+1) a_{m+1} x^m$$

Switching the dummy index back to n and rearranging the terms in (3.12) we get

$$\sum_{n=0}^{\infty} \left[(n+1) a_{n+1} - a_n \right] x^n = 0$$

In order for this equation to be valid for all values of x, we therefore require

$$a_{n+1} = \frac{1}{n+1} a_n$$

This is the "recursion relation" mentioned above. It tells us how to get any coefficient in terms of the one before. If we set $a_0 = c$ then it is clear that

$$a_1 = \frac{1}{1} c \qquad a_2 = \frac{1}{2} a_1 = \frac{1}{2 \cdot 1} c \qquad a_3 = \frac{1}{3} a_2 = \frac{1}{3 \cdot 2 \cdot 1} c$$

and so forth. In other words, $a_n = c/n!$ for all n. The resulting solution is

$$y(x) = \sum_{n=0}^{\infty} \frac{1}{n!} c x^n = c \sum_{n=0}^{\infty} \frac{1}{n!} x^n = ce^x$$

and indeed we get the solution we expected.

We'll do one more simple example to see how this works for a second order equation. Let's use the series approach to find the solution to

$$y''(x) = -y(x)$$

which we know to be $y(x) = c_1 \cos x + c_2 \sin x$. Substituting the series form and doing the same manipulations as before ends up with

$$\sum_{n=0}^{\infty} \left[(n+2)(n+1) a_{n+2} + a_n \right] x^n = 0 \qquad \text{so} \qquad a_{n+2} = -\frac{1}{(n+2)(n+1)} a_n$$

This time, the recursion relation skips over the prior term, which means that we are free to specify both a_0 and a_1. Writing $a_0 = c_1$ and $a_1 = c_2$ we get

$$a_2 = -\frac{1}{2\cdot 1}c_1 \qquad a_4 = -\frac{1}{4\cdot 3}a_2 = +\frac{1}{4!}c_1 \quad \cdots \quad \text{so} \quad a_{2n} = (-1)^n\frac{1}{n!} \quad \text{for} \quad n = 0, 1, 2, 3, \ldots$$
$$a_3 = -\frac{1}{3\cdot 2}c_2 \qquad a_5 = -\frac{1}{4\cdot 4}a_3 = +\frac{1}{5!}c_2 \quad \cdots \quad \text{so} \quad a_{2n+1} = (-1)^n\frac{1}{n!} \quad \text{for} \quad n = 0, 1, 2, 3, \ldots$$

The solution naturally separates into two series, namely

$$\begin{aligned} y(x) &= c_1\left[1 - \frac{1}{2!}x^2 + \frac{1}{4!}x^4 + \cdots\right] + c_2\left[x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 + \cdots\right] \\ &= c_1\cos x + c_2\sin x \end{aligned}$$

and once again we get the correct solution.

Many physical problems result in second order linear ODE's whose solutions can only be written in terms of series. Many of these solutions are given special names. A few of the most important examples are discussed in Section 3.6.

3.5.2 The quantum mechanical simple harmonic oscillator

Quantum Mechanics can be formulated in terms of differential equations. In particular, the Schrödinger Equation is an approach to Quantum Mechanics where one solves for the *wave function* $\psi(x)$ for a particle of mass m acted on by a potential energy function $V(x)$ by solving the differential equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$$

subject to some boundary conditions. For solutions that are localized in some region of x, so-called "bound state solutions", it turns out that solutions are only possible for discrete values of the total energy E. That is, the energies are "quantized", hence the name of this field. The boundary conditions do not typically make it possible to find all of the integration parameters, but an additional *normalization* constraint is included, namely that the integral of $|\psi(x)|^2$ over all x must equal unity. This allows $|\psi(x)|^2$ to be interpreted as a "probability density."

Let's take on the solution for the simple harmonic oscillator, where $V(x) = kx^2/2 = m\omega_0^2x^2/2$ is the potential energy function. (We know from our past work that $\omega_0^2 = k/m$ is a useful parameter, so let's put it in at the start.) The differential equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega_0^2x^2\psi(x) = E\psi(x)$$

The function $\psi(x)$ is subject to the boundary condition that $\psi(x \to \pm\infty) = 0$.

First, it is a good idea to change variables from x to y equal to x divided by some length scale. Since finding the energy will be part of the problem, let's not use E to find a length scale, and instead form it out of $\hbar$, m, and ω_0. Writing the length scale as $\hbar^x m^y \omega_0^z$, we need

$$L = [\hbar]^x \cdot [m]^y \cdot [\omega_0]^z = L^{2x} M^x T^{-x} \cdot M^y \cdot T^{-z} = L^{2x} M^{x+y} T^{-x-z}$$

so $x = 1/2$ and $y = -1/2 = z$. Therefore we write $y = x/\sqrt{\hbar/m\omega_0}$ and

$$-\frac{\hbar^2}{2m}\frac{m\omega_0}{\hbar}\frac{d^2\psi}{dy^2} + \frac{1}{2}m\omega_0^2\frac{\hbar}{m\omega_0}y^2\psi(y) = E\psi(y)$$

Multiplying through by $2/\hbar\omega_0$ and defining $\epsilon \equiv 2E/\hbar\omega_0$, and doing a little rearranging, we arrive at the second order linear homogeneous differential equation

$$\psi''(y) + (\epsilon - y^2)\psi(y) = 0 \tag{3.13}$$

This equation looks innocuous enough, but in fact its solution will take some gymnastics, even before we get to applying the series solution. Solving this will be a good illustration of how physicists make use of "flying by the seat of the pants" to come up with solutions to differential equations.

The fact that we need $\psi(y)$ to go to zero for large $\pm y$ suggests a good first step. Since ϵ is a constant, we might first consider the differential equation

$$\psi''(y) - y^2\psi(y) = 0$$

to understand the dependence on y for $y \to \pm\infty$. (We typically call this the "asymptotic dependence.") This solution to this equation is also not available in an analytic form, but if we consider the function

$$\psi(y) = e^{-y^2/2} \qquad \text{then} \qquad \psi''(y) - y^2\psi(y) = -e^{-y^2/2} \to 0 \qquad \text{as} \qquad y \to \pm\infty$$

This suggests the "asymptotic behavior" of $\psi(y)$ might behave something like $e^{-y^2/2}$. We can remove this behavior by writing

$$\psi(y) = e^{-y^2/2}h(y) \tag{3.14}$$

and then inserting this into (3.13) to find the differential equation satisfied by $h(y)$.

I admit this all sounds cockamamie. However, don't forget that existence and uniqueness are there for us, so any way that works is fine.

So let's use (3.14) in (3.13) and see what happens. The derivatives are

$$\begin{aligned}
\psi'(y) &= e^{-y^2/2}h'(y) - ye^{-y^2/2}h(y) \\
\psi''(y) &= e^{-y^2/2}h''(y) - 2ye^{-y^2/2}h'(y) + y^2e^{-y^2/2}h(y) - e^{-y^2/2}h(y)
\end{aligned}$$

Inserting this into (3.13) gives

$$e^{-y^2/2}h''(y) - 2ye^{-y^2/2}h'(y) - e^{-y^2/2}h(y) + \epsilon e^{-y^2/2}h(y) = 0$$

Dividing out the exponential factor leaves us with

$$h''(y) - 2yh'(y) + \lambda h(y) = 0 \qquad \text{where} \qquad \lambda \equiv \epsilon - 1 \tag{3.15}$$

Mathematicians have given this second order linear ODE a name, the Hermite Equation. We can use the series approach to solve this equation. Proceeding as usual we have

$$\begin{aligned} h(y) &= \sum_{n=0}^{\infty} a_n y^n \\ h'(y) &= \sum_{n=0}^{\infty} n a_n y^{n-1} \qquad \text{so} \qquad yh'(y) = \sum_{n=0}^{\infty} n a_n y^n \\ h''(y) &= \sum_{n=0}^{\infty} n(n-1) a_n y^{n-2} = \sum_{n=0}^{\infty} (n+2)(n+1) a_{n+2} y^n \end{aligned}$$

and the Hermite Equation (3.15) becomes

$$\sum_{n=0}^{\infty} \left[(n+2)(n+1)a_{n+2} - (2n-\lambda)a_n \right] y^n = 0$$

which gives the recursion relation

$$a_{n+2} = \frac{2n-\lambda}{(n+2)(n+1)} a_n \tag{3.16}$$

and we get two independent series, one with even powers of y, and one with odd powers. (There is actually some interesting Quantum Mechanics that has to do with this observation, concerning parity symmetry, but I will leave that to your Quantum Mechanics course.)

Now this solution would actually present a difficulty. Remember that we need $\psi(x) \to 0$ for $x \to \pm\infty$. It would seem that (3.14) covers this, provided that $h(y)$ does not grow too quickly. However, consider (3.16) for large values of y, where the series is dominated by $n \gg 1$. In this case $a_{n+2} \to (2n/n^2)a_n = (2/n)a_n$. For the series with even values of $n = 2m$, the series becomes something proportional to

$$\sum_{m \gg 1} \frac{1}{m!} y^{2m} = e^{y^2}$$

From (3.14), this implies that $\psi(y) \to e^{y^2/2}$ as $y \to \pm\infty$, and there is no way that we can meet the boundary condition. (We can make the same argument for the series with odd n, just by factoring out y.)

Nevertheless, there is s solution to this problem. If the recursion relation says that the series *terminates* at some value of n, then $h(y)$ is not an infinite series, but rather a polynomial of degree n. This happens if, for some n, the numerator of (3.16) vanishes. That is

$$2n - \lambda = 2n - (\epsilon - 1) = 0$$

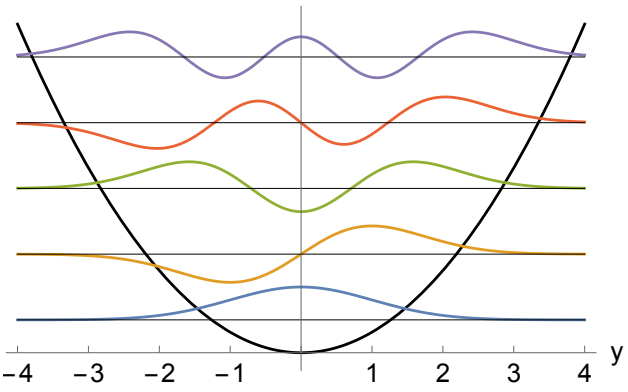


Figure 3.7: The wave functions $\psi_n(y)$ for the quantum mechanical simple harmonic oscillator, superimposed on the potential energy and energy levels. Wave functions are shown for $n = 0, 1, 2, 3, 4$ and are plotted vertically shifted so that $\psi = 0$ corresponds to the energy level $E_n = (n + 1/2)\hbar\omega_0$. Notice that $\psi_n(-y) = \psi_n(y)$ for n even, and that $\psi_n(-y) = -\psi_n(y)$ for n odd.

Since $\epsilon \equiv 2E/\hbar\omega_0$, this tells us that the allowed energies of the Quantum Mechanical Simple Harmonic Oscillator are

$$E = \frac{\hbar\omega_0}{2}(2n+1) = \left(n + \frac{1}{2}\right)\hbar\omega_0 \equiv E_n$$

The energies of the oscillator are "quantized" into evenly spaced values of $\hbar\omega_0$. This is a profound and familiar result in Quantum Mechanics, which you will see again in Physics.

For any value of n, the finite series $h_n(x)$ is called the Hermite Polynomial of order n. The wave functions $\psi(y)$ can then be written as

$$\psi(y) = N_n h_n(y) e^{-y^2/2} \equiv \psi_n(y)$$

where N_n is a "normalization constant" that is set by a different assumption of Quantum Mechanics, namely that the integral of $\psi(y)$ over all y is unity. There are ways to determine a formula for N_n, but I won't cover that here. The first five Hermite polynomials are

n	$h_n(y)$
0	1
1	$2y$
2	$4y^2 - 2$
3	$8y^3 - 12y$
4	$16y^4 - 48y^2 + 12$

Figure 3.7 shows the first five wave functions plotted on top of the energy levels. The "parity" $(-1)^n$ of the wave functions is apparent, as is the fact that $\psi_n(y) \to 0$ for $y \to \pm\infty$. In fact, the inflection point where the wave function turns to decreasing from oscillatory always occurs at the "classical turning point" where the total energy equals the potential energy.

We have only scratched the surface of this very important problem in Quantum Mechanics. You will learn more in other courses, but note the lesson here that sometimes the infinite series solution will be truncated to a polynomial. We will encounter an example of this in the next section when we discuss the Legendre Equation.

3.6 Some Important Special Functions

There are many physical situations that give rise to specific linear second order ordinary differential equations. The important ones all have names, usually based on the mathematician who popularized them and their solutions. Oftentimes, the solutions to these equations can only be expressed as infinite series, or series truncated to become polynomials. The solutions generally go by the same name as the differential equations they solve. We saw one example of this in Section 3.5.2 with the Hermite Equation and Hermite Polynomials.

Section 4.2.4 will discuss Laplacian operator $\vec{\nabla}^2$, which leads to partial differential equations in different areas of Physics. For example, $\vec{\nabla}^2 V = 0$, called Laplace's Equation, is used to derive the electric potential in the presence of static charges, along with some boundary conditions. In Quantum Mechanics, $\vec{\nabla}^2\psi = -k^2\psi$ is solved to find the wave function for a free particle with momentum $\hbar k$. These are important examples because, as we will learn later, a technique called "Separation of Variables" leads to second order ordinary differential equations in the spatial coordinates.

We call the solutions to these specific linear second order ODE's "Special Functions" and these are the subject of this section. In many cases, these functions cannot be written in closed form but instead are written as infinite series.

Of course, there is nothing "special" about these Special Functions. They are just defined in terms of the differential equations they solve. We could just as well have defined e^x as the solution to $y'(x) = y$, and $\cos x$ and $\sin x$ as the linearly independent solutions of $y''(x) = -y$, but we didn't. In this section, we will focus on the Bessel Functions of integer order $m \geq 0$ $J_m(x)$, the Spherical Bessel Functions $j_\ell(x)$ and $n_\ell(x)$, and the Legendre Polynomials $P_\ell(x)$. It turns out that $j_\ell(x)$ and $n_\ell(x)$ can be written in closed form using $\cos x$ and $\sin x$, and the Legendre Polynomials are just that, polynomials, but the $J_m(x)$ can only be written as an infinite series.

Before we get into specific special functions, however, we need to do a little more work on the general theory of second order linear ODE's.

3.6.1 Ordinary and Singular Points

We return to writing our general second order homogeneous linear ODE as

$$r(x)y''(x) + p(x)y'(x) + q(x)y(x) = 0$$

In principle, we can just write this equation as

$$y''(x) + \frac{p(x)}{r(x)}y'(x) + \frac{q(x)}{r(x)}y(x) = 0$$

but we have to be careful. For some value of $x = x_0$ at which $r(x_0) = 0$, we cannot just assume that the second equation has a solution that is the same as for the first. Such points

$x = x_0$ are called *singular points*, whereas other values of x are called *ordinary points*. If

$$\lim_{x\to x_0}(x-x_0)\frac{p(x)}{r(x)} \qquad \text{and} \qquad \lim_{x\to x_0}(x-x_0)^2\frac{q(x)}{r(x)}$$

are finite, then $x = x_0$ is called a *regular singular point*. For regular singular points, the functions $(x-x_0)p(x)/r(x)$ and $(x-x_0)^2a(x)/r(x)$ will have well behaved Taylor expansions about $x = x_0$, so a series solution approach can be pursued.

We will only be discussing solutions of this class for regular singular points. Solutions for differential equations about irregular singular points is an advanced topic that I will leave for a Mathematics course.

Let's examine two of the equations we will study in this section with respect to their singular points. First consider Bessel's Equation, namely

$$x^2y''(x) + xy'(x) + (x^2 - \nu^2)y(x) = 0 \tag{3.17}$$

Clearly, $x = 0$ is a singular point. However, since

$$\lim_{x\to 0} x\frac{x}{x^2} = \lim_{x\to 0} 1 = 1 \qquad \text{and} \lim_{x\to 0} x^2\frac{x^2-\nu^2}{x^2} = -\nu^2$$

are both finite, $x = 0$ is a regular singular point and we can go ahead and try to build a series solution for Bessel's Equation. We will do this in Section 3.6.2.

Now also consider the Legendre Equation, that is

$$(1-x^2)y''(x) - 2xy'(x) + \alpha(\alpha+1)y(x) = 0 \tag{3.18}$$

In this case there are two singular points, at $x = \pm 1$. However, since

$$\lim_{x\to 1}(x-1)\frac{-2x}{1-x^2} = \lim_{x\to 1}(x-1)\frac{-2x}{(1-x)(1+x)} = 2 \qquad \text{and} \qquad \lim_{x\to 1}(x-1)^2\frac{\alpha(\alpha+1)x}{(1-x)(1+x)} = 0$$

are both finite, $x = +1$ is a regular singular point. Similarly for $x = -1$.

Of course, if $x = x_0$ is a singular point, we can always build a series solution around a different value of x, in which case we don't need to be concerned whether the point is regular or irregular. The behavior of the solution at $x = x_0$, though, is likely to be peculiar.

Euler Equations

There is an instructive class of second order ODE's with regular singular points called Euler Equations (not to be confused with Euler's Formula from Section 2.4). Euler Equations take the form

$$x^2y''(x) + \alpha xy'(x) + \beta^2y(x) = 0$$

It should be clear that there is a regular singular point at $x = 0$. (We could write a slightly different equation with $(x - x_0)$ instead of x in front of the first and second terms, and get a regular singular point at $x = x_0$.)

It should also be clear that a series solution to this equation would not work. No recursion relation comes from inserting the series into the equation, because the powers of x in front of $y''(x)$ and $y'(x)$ bring all powers of x back up to x^n.

Nevertheless, this equation has a straightforward solution that brings to mind the ansatz we used for the second order ODE with linear coefficients. Inserting $y(x) = x^r$, where r is a constant to be determined, we get the quadratic equation

$$r(r-1) + \alpha r + \beta = r^2 + (\alpha - 1)r + \beta^2 = 0$$

which is to be solved for r. Evidently, the two solutions for r are

$$r = \frac{-(\alpha - 1) \pm \sqrt{(\alpha - 1)^2 - 4\beta^2}}{2}$$

There are three obvious cases. For $(\alpha - 1)^2 > 4\beta^2$, there are two real values $r = r_1$ and $r = r_2$ for which x^r is a solution. That is, the general solution is

$$y(x) = c_1 x^{r_1} + c_2 x^{r_2}$$

If $(\alpha - 1)^2 < 4\beta^2$, then the roots are complex, and we make use of $x^{\mu+i\eta} = e^{(\mu+i\eta)\log x}$ to write the solutions. If the two values of r are equal, we need to figure out some way to get a second equation, but I'll leave this for a homework problem.

The lesson here is that for a regular singular point, including a factor of x^r in the solution, where r is to be determined, may be a useful approach to be included in the series expansion. This approach is sometimes called the Method of Frobenius.

3.6.2 Bessel functions

A differential equation ubiquitous to physics problems is Bessel's Equation (3.17), which we reproduce here:

$$x^2 y''(x) + x y'(x) + (x^2 - \nu^2) y(x) = 0 \tag{3.19}$$

where ν is a constant, known as the *order*. As discussed above, $x = 0$ is a regular singular point, so we should pursue a series solution of the form

$$y(x) = x^r \sum_{n=0}^{\infty} a_n x^n = \sum_{n=0}^{\infty} a_n x^{r+n} \tag{3.20}$$

where we expect (3.19) to constrain r as well as determine the coefficients a_n. Inserting this form into Bessel's Equation gives us

$$\sum_{n=0}^{\infty} \left\{ \left[(r+n)(r+n-1) + (r+n) - \nu^2 \right] a_n x^{r+n} + a_n x^{r+n+2} \right\} = 0 \tag{3.21}$$

Notice that we would be in trouble if we didn't include the factor x^r. Setting $r = 0$ gives

$$\sum_{n=0}^{\infty} \left\{ (n^2 - \nu^2) a_n x^n + a_n x^{n+2} \right\} = 0$$

which implies that $a_0 = 0$ and $a_1 = 0$, based on the x^0 and x^1 terms. Deriving a recursion relation gives a_{n+2} in terms of a_n, so all the a_n end up as zero. This would all be nonsense!

We can simplify (3.21) to get

$$\sum_{n=0}^{\infty} \left\{ \left[(r+n)^2 - \nu^2 \right] a_n x^{r+n} + a_n x^{r+n+2} \right\} = 0 \tag{3.22}$$

In this case, for the x^0 term, we have $r^2 - \nu^2 = 0$ which gives us two possibilities for r, namely $r = \pm\nu$. Setting the coefficient of the x^1 term to zero gives

$$[(r+1)^2 - \nu^2] a_1 = [(\pm 2\nu + 1] a_1 = 0$$

which implies that $a_1 = 0$, unless $\nu = \pm 1/2$, a case we will deal with in Section 3.6.3.

It should be clear that we indeed get two solutions for $y(x)$, one each for $r = \pm\nu$. Following the recursion relation we will derive from (3.22) results in the two functions we call $J_{\pm\nu}(x)$, known as *Bessel Functions of the first kind.* The theory associated with Bessel Functions is extensive, but we will not go very far into it. Nearly all cases in Physics that involve Bessel Functions result in functions where ν is either a positive integer, or a positive half-integer.

At this point, we will specialize to the case where $\nu = m \in \mathbb{Z}$, an integer. I will tell you at the outset, but not prove, that for this case, the solutions $J_m(x)$ and $J_{-m}(x)$ are *not* linearly independent. A different solution cam be identified, though, usually written as $Y_m(x)$ and called the *Bessel Function of the Second Kind*, which is independent. I am leaving this very interesting Mathematics for some later course you will hopefully take.

With the first two terms of the sum being zero, we can rewrite the first term in curly brackets in (3.22) as

$$x^m \left\{ \sum_{n=2}^{\infty} \left[(m+n)^2 - m^2 \right] a_n x^n \right\} = x^m \left\{ \sum_{p=0}^{\infty} \left[(m+p+2)^2 - m^2 \right] a_{p+2} x^{p+2} \right\}$$

where we switch to the dummy index $p = n - 2$. Switching p back n, we replace the above expression in (3.22) and divide out x^m to get

$$\sum_{n=0}^{\infty} \left\{ \left[(m+n+2)^2 - m^2 \right] a_{n+2} + a_n \right\} x^{n+2} = 0$$

giving us the recursion relation

$$a_{n+2} = -\frac{1}{(m+n+2)^2 - m^2} a_n = -\frac{1}{(n+2)(2m+n+2)} a_n$$

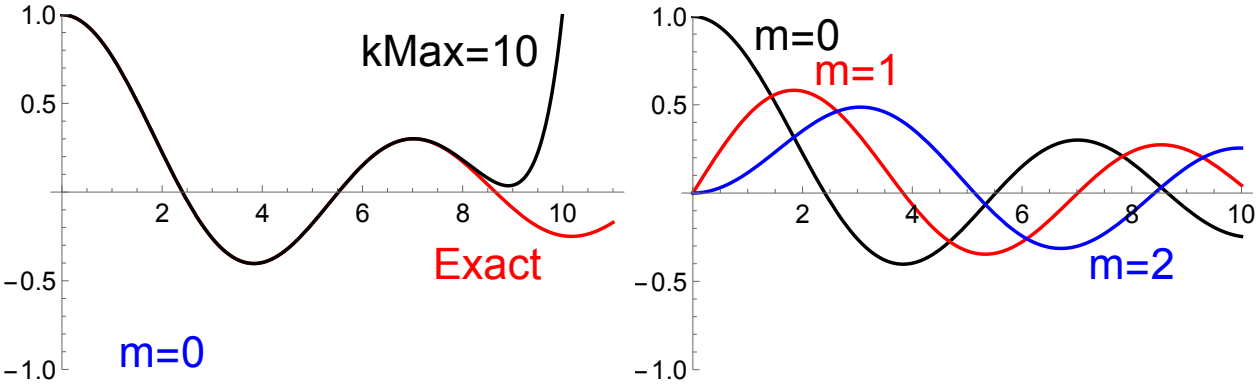


Figure 3.8: Plots of Bessel Functions $J_m(x)$ for integer orders m. The left is for $m = 0$, where the black curve uses (3.24) summing up to $k = 10$. The right curve is the "exact" $J_0(x)$ using the BesselJ function in MATHEMATICA. On the right are $J_0(x)$, $J_1(x)$, and $J_2(x)$.

Since $a_1 = 0$, the sum is only over even n. Therefore we define $n = 2k$ and sum over all integers $k \geq 0$. The recursion relation becomes

$$a_{k+1} = -\frac{1}{(2k+2)(2m+2k+2)}\, a_k = -\frac{1}{(k+1)(m+k+1)}\, a_k\, \frac{1}{2^2} \tag{3.23}$$

These coefficients are to be inserted into (3.20) which we now write as

$$J_m(x) = \sum_{k=0}^{\infty} a_k x^{m+2k}$$

By convention, we write $a_0 = 1/m!2^m$ and therefore

$$\begin{aligned} a_1 = \frac{(-1)}{(1)(m+1)} a_0 \frac{1}{2^2} &= \frac{(-1)}{(1)(m+1)!}\, \frac{1}{2^{m+2}} \\ a_2 = \frac{(-1)}{(2)(m+2)} a_1 \frac{1}{2^2} &= \frac{(-1)^2}{(2\cdot 1)(m+2)!}\, \frac{1}{2^{m+4}} \\ \text{that is} \qquad a_k &= \frac{(-1)^k}{(k!)(m+k)!}\, \frac{1}{2^{m+2k}} \end{aligned}$$

Finally, then, we arrive at the series expansion for the Bessel Function of integer order as

$$J_m(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(m+k)!} \left(\frac{x}{2}\right)^{m+2k} \qquad m = 0, 1, 2, 3, \ldots \tag{3.24}$$

Figure 3.8 shows on the left $J_0(x)$ using (3.8) summing over $k = 0, 1, \ldots, 10$. The function oscillates with decreasing amplitude, but diverges near $x = 9$. This is not surprising, given that the polynomial grows rapidly when the last term is proportional to x^{10}.

Of course, nobody ever uses (3.8) explicitly to calculate Bessel Functions. The theory of Bessel Functions provides a number of useful algorithms for calculating $J_m(x)$ to high precision for any x. The left plot of Figure 3.8 also shows $J_0(x)$ as calculated by the internal function in MATHEMATICA. The right plots the first three integer order Bessel Functions $J_0(x)$, $J_1(x)$, and $J_2(x)$. Note how the behavior near $x = 0$ closely tracks x^m.

3.6.3 Spherical Bessel functions

A very common (partial) differential equation in Physics is the Helmholtz Equation, namely

$$\vec{\nabla}^2 u(\mathbf{r}) + k^2 u(\mathbf{r}) = 0 \tag{3.25}$$

where $u(\mathbf{r})$ is a function in three dimensional space of the coordinate $\mathbf{r}$. We will study this equation in Section 4.2.4. For now, however, what is important to realize is the when we solve this equation in spherical coordinates, the ordinary differential equation

$$r^2 R''(r) + 2rR'(r) + \left[k^2 r^2 - \ell(\ell+1)\right] R(r) = 0 \tag{3.26}$$

where ℓ is a non-negative integer. This equation needs to be solved for $R(r)$, where $r = |\mathbf{r}|$. If we switch to a (dimensionless) variable $x = kr$, and write $R(r) = x^{-1/2} y(x)$, then

$$\begin{aligned}
R'(r) &= \frac{dR}{dr} = k\frac{d}{dx}\left[x^{-1/2} y(x)\right] = k\left[\frac{y'(x)}{x^{1/2}} - \frac{1}{2}\frac{y(x)}{x^{3/2}}\right] \\
2rR'(r) &= 2x^{1/2} y'(x) - \frac{y(x)}{x^{1/2}} \\
R''(r) &= \frac{d}{dr}R'(r) = k\frac{d}{dx}\left\{k\left[\frac{y'(x)}{x^{1/2}} - \frac{1}{2}\frac{y(x)}{x^{3/2}}\right]\right\} = k^2\left[\frac{y''(x)}{x^{1/2}} - \frac{y'(x)}{x^{3/2}} + \frac{3}{4}\frac{y(x)}{x^{5/2}}\right] \\
r^2 R''(r) &= x^{3/2} y''(x) - x^{1/2} y'(x) + \frac{3}{4}\frac{y(x)}{x^{1/2}}
\end{aligned}$$

Inserting this into (3.26) and multiplying through by $x^{1/2}$ gives

$$x^2 y''(x) + xy'(x) - \frac{1}{4}y(x) + \left[x^2 - \ell(\ell+1)\right] y(x) = 0$$

Now $\ell(\ell+1) + 1/4 = \ell^2 + \ell + 1/4 = (\ell + 1/2)^2$ so we finally have

$$x^2 y''(x) + xy'(x) + \left[x^2 - \left(\ell + \frac{1}{2}\right)^2\right] y(x) = 0 \tag{3.27}$$

which is Bessel's Equation for $\nu = \ell + 1/2$. Therefore, solutions to (3.27) are of the form

$$y(x) = c_1 J_{\ell+1/2}(x) + c_2 Y_{\ell+1/2}(x)$$

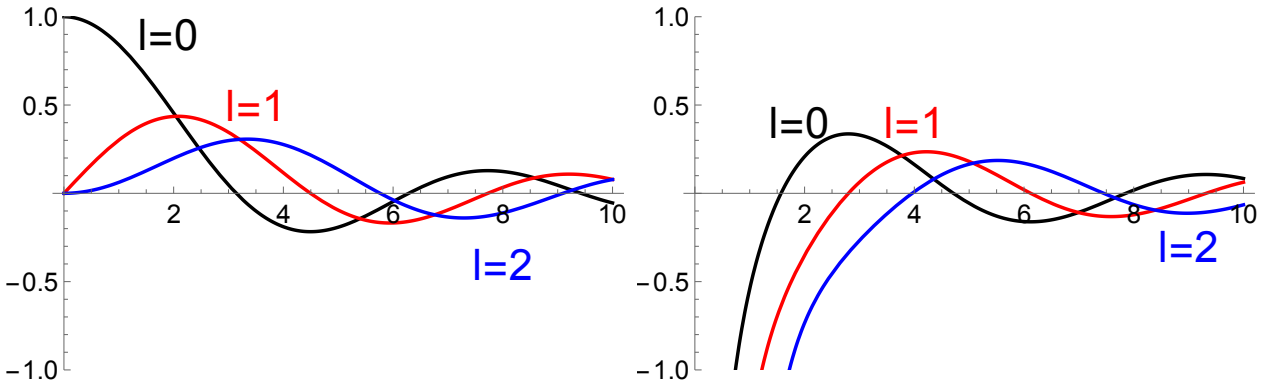


Figure 3.9: The Spherical Bessel Functions $j_\ell(x)$ (left) and $n_\ell(x)$ (right) for $\ell = 0, 1, 2$.

Of course, physically, we are interested in $R(r) = (kr)^{-1/2}y(kr)$, so it is customary to define

$$j_\ell(x) \equiv \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x) \tag{3.28a}$$

$$\text{and} \qquad n_\ell(x) \equiv \sqrt{\frac{\pi}{2x}} Y_{\ell+1/2}(x) \tag{3.28b}$$

These are known as the *Spherical Bessel Functions*. It is not very difficult to show that

$$j_0(x) = \frac{\sin x}{x} \qquad \text{and} \qquad n_0(x) = -\frac{\cos x}{x}$$

and that there is a recurrence relation for the higher orders, namely

$$f_\ell(x) = (-1)^\ell x^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell f_0(x)$$

where $f_\ell(x)$ can be either $j_\ell(x)$ or $n_\ell(x)$. It is interesting note that $j_\ell(x)$ and $n_\ell(x)$, unlike the $J_\nu(x)$, can be written in terms of sine and cosine functions.

Figure 3.9 plots $j_\ell(x)$and $n_\ell(x)$ for the three lowest values of ℓ. The $n_\ell(x)$ are singular for $x \to 0$, but you are much more likely to encounter the $j_\ell(x)$ in future Physics course. The most important Physics application I'm aware of, for the $n_\ell(x)$, have to do with scattering problems in Quantum Mechanics.

3.6.4 Legendre polynomials

In physical problems involving the Helmholtz Equation (3.25) where the system has spherical symmetry, that is $u(\mathbf{r}) = u(r)$, you encounter the Legendre Equation

$$(1 - x^2)y''(x) - 2xy'(x) + \ell(\ell + 1)y(x) = 0 \tag{3.29}$$

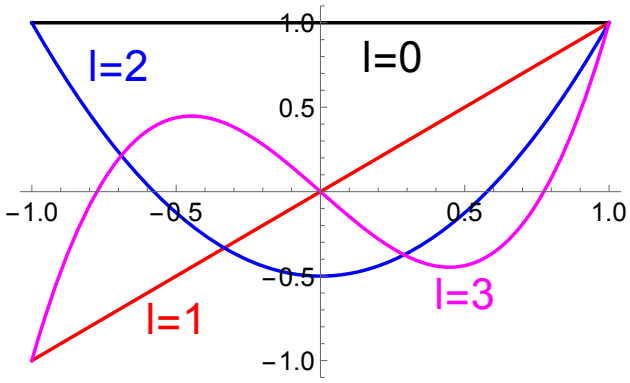


Figure 3.10: The first four Legendre Polynomials $P_0(x)$, $P_1(x)$, $P_2(x)$, and $P_3(x)$,

where $x = \cos\theta$ is defined in terms of the polar angle $0 \le \theta \le \pi$. For most physical problems of interest, ℓ is a non-negative integer, that is, $\ell = 0, 1, 2, \ldots$.

Legendre's Equation has regular singular points at $x = \pm 1$, but not at $x = 0$, so the simple series approach, setting

$$y = \sum_{n=0}^{\infty} a_n x^n$$

should work fine. Substituting this into (3.29) gives

$$\sum_{n=0}^{\infty} \left\{ n(n-1)a_n x^{n-2} + \left[-n(n-1) - 2n + \ell(\ell+1) \right] a_n x^n \right\} = 0$$

which results in the recursion relation

$$a_{n+2} = \frac{n(n-1) + 2n - \ell(\ell+1)}{(n+2)(n+1)}\, a_n = \frac{n(n+1) - \ell(\ell+1)}{(n+2)(n+1)}\, a_n$$

The free parameters are therefore a_0 and a_1, and these determine the two series, one with only even powers of x, and one with only odd powers.

Clearly, $a_{\ell+2} = 0$ for any given ℓ, so the solutions to (3.29) are polynomials of degree ℓ, called Legendre Polynomials $P_\ell(x)$. By convention, we set $P_\ell(1) = 1$, and this fixes a_0 and a_1.

The first few Legendre Polynomials are

$$\begin{array}{ll} P_0(x) = 1 & P_1(x) = x \\ P_2(x) = \frac{1}{2}(3x^2 - 1) & P_3(x) = \frac{1}{2}(5x^3 - 3x) \\ P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3) & P_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x) \end{array}$$

Figure 3.10 plots the Legendre Polynomials for $\ell = 0$, $\ell = 1$, $\ell = 2$, and $\ell = 3$. These solutions to (3.29) can also be written as

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dx^\ell} (x^2 - 1)^\ell \tag{3.30}$$

known as Rodrigues' Formula.

Associated Legendre functions

Maybe just show what they are. Can it be an exercise to show that they solve the appropriate differential equation?

3.6.5 Laguerre polynomials

These show up in the solution to the hydrogen atom in quantum mechanics. Probably not enough time to go into this, though.

3.6.6 The confluent hypergeometric function

Very cool, but probably can't cover it. Maybe a homework problem.

3.7 Coupled Differential Equations

It is possible, and physically likely, that a system will be governed by more than one differential equation, for more than one dependent variable, and that these dependent variables appear in more than one of the equations. In this case, we say that the differential equations are *coupled*. In general, for these cases, we will have to be clever in order to find a solution, even if the equations are linear and homogeneous. Remember, for the purposes of this course, at least, we are guided by existence and uniqueness.

Rather than try to treat coupled differential equations in general, we will take the opportunity to solve a specific problem, namely the motion of coupled simple harmonic oscillators. We will see that generalizing the ansatz we used for the oscillator will set us in the right direction. It will also provide hints to the concept of *eigenvalues*, which we will cover more thoroughly in Section 6.4.

3.7.1 Coupled Simple Harmonic Oscillators

Figure 3.11 shows a prototype of coupled linear second order differential equations. Two masses m_1 and m_2 are each attached by springs to a fixed wall. They are also connected by a "coupling" spring, and the force on each mass due to the coupling spring depends on the positions of each of the masses. Note that the force the coupling spring exerts on m_1 is equal and opposite to the force it exerts on m_2. Newton's Second Law, applied separately to the two masses, becomes

$$\begin{aligned} m_1\ddot{x} = F_1 &= -k_1x_1 + k_2(x_2 - x_1) \\ m_2\ddot{x} = F_2 &= -k_3x_2 - k_2(x_2 - x_1) \end{aligned}$$

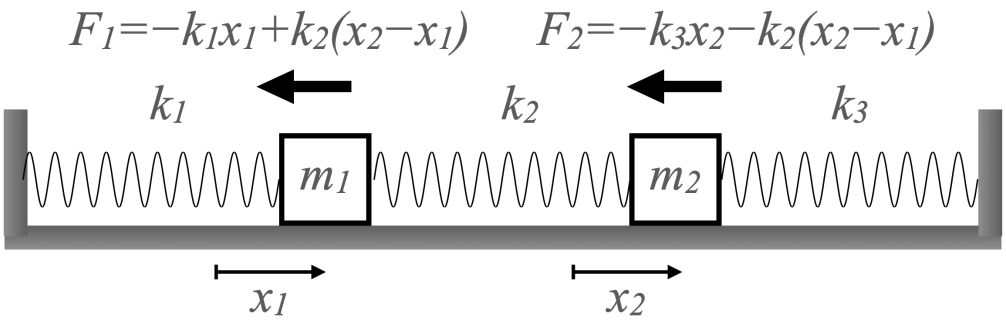


Figure 3.11: A coupled harmonic oscillator with two masses and three springs.

If you have trouble seeing the sign on the coupling force, just think about what happens if m_2 is extended more than m_1 in which case the spring wants to compress, moving m_1 to the right and m_2 to the left.

At this point we will make the problem even more specific, and set $m_1 = m_2 = m$ and $k_1 = k_2 = k_3$. Defining $\omega_0^2 = k/m$, we get the differential equations

$$x_1''(t) + 2\omega_0^2 x_1(t) - \omega_0^2 x_2(t) = 0 \tag{3.31a}$$
$$x_2''(t) + 2\omega_0^2 x_2(t) - \omega_0^2 x_1(t) = 0 \tag{3.31b}$$

These differential equations are clearly "coupled." The equation for $x_1(t)$ depends on the function $x_2(t)$, and the equation for $x_2(t)$ depends on the function $x_1(t)$.

We will approach the solution using the ansatz

$$x_1(t) = a_1 e^{i\omega t} \qquad \text{and} \qquad x_2(t) = a_2 e^{i\omega t}$$

and look to see what we can learn about ω, a_1, and a_2. This ansatz would seem to imply that both masses oscillate at the same frequency ω. However, let's plow forward and see what happens. Inserting this ansatz into (3.31) we have

$$\begin{aligned} -\omega^2 a_1 + 2\omega_0^2 a_1 - \omega_0^2 a_2 &= 0 \\ -\omega^2 a_2 + 2\omega_0^2 a_2 - \omega_0^2 a_1 &= 0 \end{aligned}$$

Let me rewrite these equations in a suggestive form, and that will become more clear to you when we cover systems of linear equations in Section 6.3.9. We have

$$(2\omega_0^2 - \omega^2)a_1 - \omega_0^2 a_2 = 0 \tag{3.32a}$$
$$-\omega_0^2 a_1 + (2\omega_0^2 - \omega^2)a_2 = 0 \tag{3.32b}$$

One obvious solution to these equations is $a_1 = a_2 = 0$, but that just means that neither mass ever moves. There would also be no way to accommodate arbitrary initial conditions for position and velocity one each of the masses. Our notions of existence and uniqueness tell us that there has to be another way to solve these equations.

Remember that we have ω^2 to play with. If ω^2 was set to some value that made both equations the *same* equation, then all we could get out of this would be constraints on the ratio of a_1/a_2, in which case we can use initial conditions to solve the rest of the problem. The two equations (3.32) become one equation if the coefficients of a_1 and a_2 are in the same ratio, that is

$$\frac{2\omega_0^2 - \omega^2}{-\omega_0^2} = \frac{-\omega_0^2}{2\omega_0^2 - \omega^2}$$

This equation is simple to solve for ω^2. We get

$$(2\omega_0^2 - \omega^2)^2 = \omega_0^4 \qquad \text{so} \qquad \omega^2 = 2\omega_0^2 \pm \omega_0^2 = \omega_0^2,\, 3\omega_0^2$$

Indeed, there are two frequencies ω for which the two masses can oscillate together. Of course, the real solution can be any linear combination of these solutions, each of which is proportional to $e^{\pm i\omega t}$. There is an important constraint on these solutions, though, namely the ratio of a_1 and a_2 that comes from (3.32). In the case where $\omega^2 = \omega_0^2$, we find

$$\omega_0^2 a_1 - \omega_0^2 a_2 = 0 \qquad \text{so} \qquad a_2 = a_1 \qquad \text{where} \qquad \omega^2 = \omega_0^2$$

while for $\omega^2 = 3\omega_0^2$,

$$-\omega_0^2 a_1 - \omega_0^2 a_2 = 0 \qquad \text{so} \qquad a_2 = -a_1 \qquad \text{where} \qquad \omega^2 = 3\omega_0^2$$

In other words, if the two masses are going to oscillate at the same frequency, then they either follow each other with the same amplitude and phase (at frequency $\omega = \omega_0$) or they follow each other with the same amplitude but 180° out of phase (at frequency $\omega = \sqrt{3}\omega_0$).

The general solution can now be written in terms of the four constants a, b, c, and d as

$$x_1(t) = ae^{i\omega_0 t} + be^{-i\omega_0 t} + ce^{i\sqrt{3}\omega_0 t} + de^{-i\sqrt{3}\omega_0 t} \tag{3.33a}$$

$$x_2(t) = ae^{i\omega_0 t} + be^{-i\omega_0 t} - ce^{i\sqrt{3}\omega_0 t} - de^{-i\sqrt{3}\omega_0 t} \tag{3.33b}$$

The constants are determined from the initial conditions on $x_1(0)$, $\dot{x}_1(0)$, $x_2(0)$, and $\dot{x}_2(0)$. I urge you to take the time to insert (3.32) into (3.32) and confirm that these are in fact solutions for any a, b, c, and d.

Notice that, regardless of the initial conditions, the linear combination $x_+(t) \equiv x_1(t) + x_2(t)$ oscillates at the frequency ω_0, while the linear combination $x_-(t) \equiv x_1(t) - x_2(t)$ oscillates at the frequency $\sqrt{3}\omega_0$. In Chapter 6 we will learn to call ω_0^2 and $3\omega_0^2$ *eigenvalues*, and the solutions $x_\pm(t)$ will be components of *eigenvectors*. Somewhat more colloquially, we'll call the two kinds of motion associated with $x_\pm(t)$ "eigenmodes."

It is straightforward to take the four equations

$$x_1(0) = x_{1_0} \qquad \dot{x}_1(0) = v_{1_0} \qquad x_2(0) = x_{2_0} \qquad \dot{x}_2(0) = v_{2_0}$$

and solve for a, b, c, and d, so I won't bother to write it out. (Of course, you can just feed this into MATHEMATICA and let it solve the equations for you.) Figure 3.12 shows the

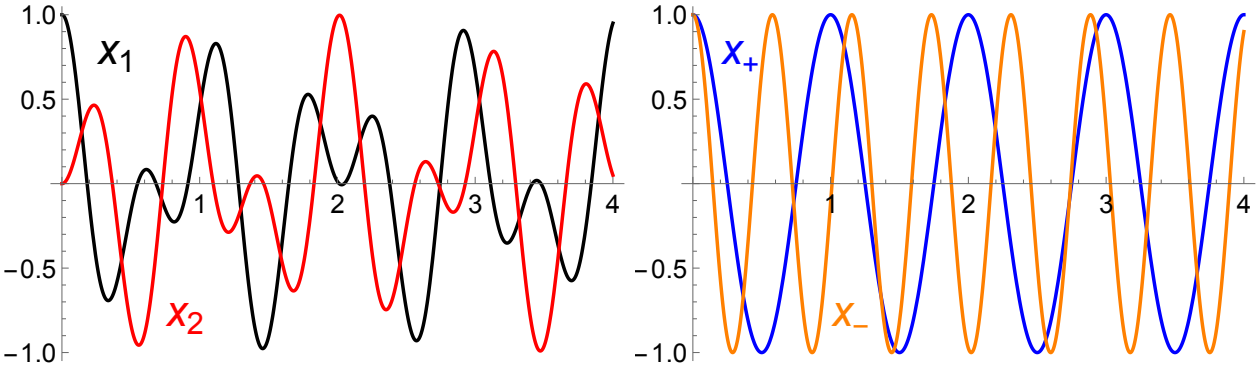


Figure 3.12: Left: The motions $x_1(t)$ and $x_2(t)$ for initial conditions $x_1(0) = 1$ and $x_2(0) = \dot{x}_1(0) = \dot{x}_2(0) = 0$, plotted as a function of time in units of $2\pi/\omega_0$. Right: Plots of $x_+(t) \equiv x_1(t) + x_2(t)$ and $x_-(t) \equiv x_1(t) - x_2(t)$.

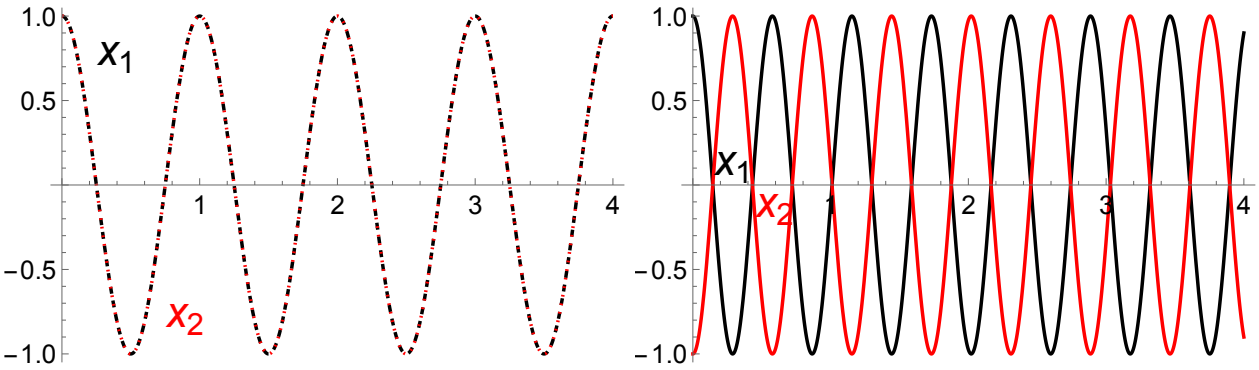


Figure 3.13: The motions $x_1(t)$ and $x_2(t)$ for initial condition variables $x_{1_0} = 1$ and $x_{2_0} = 1$ (left) and $x_{1_0} = 1$ and $x_{2_0} = -1$ (right). (The initial velocities are still $v_{1_0} = v_{2_0} = 0$.)

motions $x_1(t)$ and $x_2(t)$ for initial condition variables $x_{1_0} = 1$ and $x_{2_0} = v_{1_0} = v_{2_0} = 0$. Time is measured here in units of $2\pi/\omega_0$. The motion is periodic, although not purely harmonic. Indeed, these motions are the mixture of two frequencies, namely ω_0 and $\sqrt{3}\omega_0$.

Figure 3.12 also plots $x_+(t)$ and $x_-(t)$, which now show clearly the two fundamental frequencies of this two-body coupled system.

It is not hard to set the two masses in motion so that they oscillate each at the same frequency. All we need to do is set the initial conditions to respect the relationships between the two amplitudes for the frequency eigenvalue in question. This is shown in Figure 3.13 where we set $x_2(0) = x_1(0)$ on the left, resulting in both oscillating together at frequency ω_0 - note that the period of oscillation is clearly equal to unity (in units of $2\pi/\omega_0$). The figure also shows that when $x_2(0) = -x_1(0)$, the two masses again oscillate together, but now at frequency $\sqrt{3}\omega_0$.

3.8 Green's Functions

There is a nice treatment in Section 4.6 in Nearing's book. There will not likely be enough time to cover this, though.

Chapter 4

Vector Calculus and Partial Differential Equations

This chapter focuses on *vectors* as entities which describe quantities in ordinary three dimensional space. We'll talk a little bit about generalizing what we mean by a "vector" in Section 4.1.4, but will take this generalization much further in Chapter 6.

4.1 Vectors as Spatial Variables

Your first introduction to a "vector" was probably something written like $\vec{r}$ which stood for three (real number) values, likely called x, y, and z, and which located a point in three dimensional space. A very simple form might have been $\vec{r} = (x, y, z)$, and this tells the position of the point by marking off the distance on the x-, y-, and z-axes. However, we will be more sophisticated than this, and write

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k} \tag{4.1}$$

where $\hat{i}$, $\hat{j}$, and $\hat{k}$ are *unit vectors* in the x-, y-, and z-directions. I'll be more precise about what I mean by "unit vector" when we talk about the *inner product* in Section 4.1.2. For now, though, just think of $\hat{i}$, $\hat{j}$, and $\hat{k}$ as dimensionless quantities of magnitude unity, but with a direction that is their respective axis.

Oftentimes, we are concerned only with vectors in a plane. In this case, the "z-component" of the vector is irrelevant for the problem at hand. Typically, we simply ignore it, although we may at some point need to refer to "the direction perpendicular to the plane" of whatever are the more relevant variables.

More generally, a vector $\vec{A}$ will be regarded as an element of $\mathbb{R}^2$ or $\mathbb{R}^3$ which represents some physical quantity in two-dimensional or three-dimensional space. Equation (4.1) is just one example. In fact, if it represents the physical location of some object that can move with

time, then another obvious vector is the velocity, namely

$$\vec{v}(t) = \frac{d\vec{r}}{dt} = \frac{dx}{dt}\hat{i} + \frac{dy}{dt}\hat{j} + \frac{dz}{dt}\hat{k}$$

Notice that I slipped it by you here that the unit vectors themselves do not change with time, which is true for this coordinate system, but not for some others. Of course, the next step would be to define the acceleration vector $\vec{a} = d\vec{v}/dt$. In general, we denote the components of a vector $\vec{A}$ as A_x, A_y, and A_z, and write

$$\vec{A} = A_x\hat{i} + A_y\hat{j} + A_z\hat{k} \tag{4.2}$$

The *magnitude*, or "length" of a vector $\vec{A} = A_x\hat{i} + A_y\hat{j} + A_z\hat{k}$ is

$$|\vec{A}| = \sqrt{A_x^2 + A_y^2 + A_z^2} \tag{4.3}$$

which of course is a positive real number. It makes sense, therefore, to borrow the notation $|\vec{A}|$ from the "magnitude" or a real or complex number. Very often, we will just write $A = |\vec{A}|$ if the context is clear. We will see a more formal way to define the magnitude of a vector when we study inner products in Section 4.1.2.

It happens often in Physics that a vector $\vec{A}$ represents some physical quantity that could have different values at different points $\vec{r}$ in space, or even at different times. In other words, we have $\vec{A} = \vec{A}(\vec{r}) = \vec{A}(x, y, z)$ or $\vec{A} = \vec{A}(\vec{r}, t) = \vec{A}(x, y, z, t)$. In this case, we refer to $\vec{A}$ as a *vector field*. Probably the first examples that come to mind are the electric field $\vec{E}$ and magnetic field $\vec{B}$, but there are many other examples, including many that do not come from electromagnetism. For example, a compressible fluid will have a "velocity field" $\vec{v} = \vec{v}(\vec{r}, t)$ that would be governed by the theory of fluid mechanics.

We could also have a so-called "scalar field" which depends on position $\vec{r}$ (and possibly time t), although the use of the term "scalar" needs some consideration that we'll deal with later. We will soon be discussing "vector differential operators" which can turn a scalar field into a vector field, in exactly the same way that the static electric field $\vec{E}(\vec{r})$ can be derived from a static electric potential $\Phi(\vec{r})$.

We have been locating position in this section by representing $\vec{r}$ by the real numbers x, y, and z. These are referred to as "Cartesian coordinates." (I think this is because they were invented by the philosopher and mathematician René Descartes.) Likewise, $\hat{i}$, $\hat{j}$, and $\hat{k}$ are "Cartesian unit vectors." However, there are other ways to locate a point in two- or three-dimensional space, namely be identifying the distance from the origin and then using one or two angles to tell the direction of the point with respect to the x-, y-, and z-axes. We will discuss these in Section 4.1.3.

First, however, we will say a few words about rotations, just to put the notion of vectors into the context that we'll eventually use to more precisely define them. Then we'll discuss two important geometrical concepts of vectors.

4.1.1 Axis rotations

It doesn't matter, of course, what direction we pick when we define our Cartesian coordinate system. If the problem has some specific direction in it, for example the direction of an electric or magnetic field, then we often choose that direction to define one of the axes, typically the z-axis. In that case, the x-axis is chosen in some direction perpendicular to z, and this defines y in a way that makes the coordinate system "right handed." (This will be more precisely defined in Section 4.1.2.)

Regardless of our choice, however, we can always do physics in some set of axes $x'y'z'$ that are rotated with respect to xyz. This rotation can be specified in any number of ways, but will typically involve three angles. (In rigid body classical mechanics, and in the theory of angular momentum in quantum mechanics, these three angles are called *Euler Angles*.) When we study matrix operations in Section 6.3 we will see that matrices with certain properties are a handy way to describe rotations, and these matrices form a *group*.

For now, though, it's just important to realize that if we write some vector as

$$\begin{aligned} \vec{A} &= A_x\hat{i} + A_y\hat{j} + A_z\hat{k} \\ \text{or} \qquad &= A_{x'}\hat{i}' + A_{y'}\hat{j}' + A_{z'}\hat{k}' \end{aligned}$$

then it is still the same vector, even though the magnitudes of the components A_x, A_y, and A_z do not need to be the same in the "primed" coordinate system, that is $A_{x'}$, $A_{y'}$, and $A_{z'}$.

4.1.2 Inner product and cross product

The *inner product*, also known as the *scalar product* or the *dot product*, of two vectors $\vec{A}$ and $\vec{B}$ is a geometric quantity. I will define it as the product of the magnitude of $\vec{A}$ times the magnitude of $\vec{B}$ times the cosine of the angle ψ between them. That is

$$\vec{A} \cdot \vec{B} = |\vec{A}||\vec{B}| \cos\psi \tag{4.4}$$

A simple interpretation of this formula is that the dot product is the projection of $\vec{A}$ in the direction of $\vec{B}$. See Figure 4.1. (Equivalently, we could say the dot product is the projection of $\vec{B}$ in the direction of $\vec{A}$.) This makes it very clear that the value of $\vec{A} \cdot \vec{B}$ has nothing to do with the coordinate system being used, including the possibility of a rotated set of Cartesian axes.

An obvious byproduct of this definition is that the inner product of a vector with itself is the square of its magnitude, that is

$$\vec{A} \cdot \vec{A} = |\vec{A}|^2$$

If we apply this to unit vectors, then it is clear that the inner product of any unit vector with itself is unity. For example

$$\hat{i} \cdot \hat{i} = 1 = \hat{j} \cdot \hat{j} = \hat{k} \cdot \hat{k} = \hat{r} \cdot \hat{r} = \hat{\phi} \cdot \hat{\phi} = \hat{\theta} \cdot \hat{\theta}$$

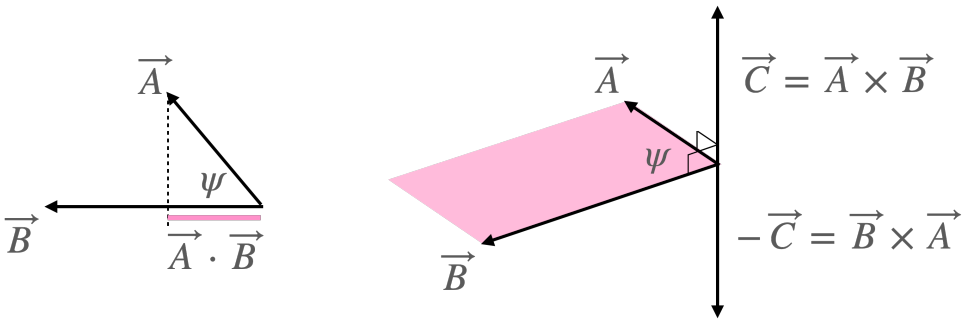


Figure 4.1: Geometric interpretations of the dot product $\vec{A} \cdot \vec{B}$ (left) and the cross product $\vec{A} \times \vec{B}$ (right) for two vectors $\vec{A}$ and $\vec{B}$. The angle between the two vectors is ψ.

Another obvious by product is that if two vectors $\vec{A}$ and $\vec{B}$ are perpendicular to each other, that is $\psi = 90°$, then $\vec{A} \cdot \vec{B} = 0$. In this case, we say that $\vec{A}$ and $\vec{B}$ are *orthogonal* to each other.

Now the unit vectors are all at 90° with respect to each other, in a given coordinate system. That is, they are orthogonal to each other. Mathematically,

$$\begin{aligned} 0 &= \hat{i} \cdot \hat{j} = \hat{j} \cdot \hat{k} = \hat{k} \cdot \hat{i} && \text{Cartesian} \\ 0 &= \hat{r} \cdot \hat{\phi} = \hat{\phi} \cdot \hat{k} = \hat{k} \cdot \hat{r} && \text{Cylindrical} \\ 0 &= \hat{r} \cdot \hat{\theta} = \hat{\theta} \cdot \hat{\phi} = \hat{\phi} \cdot \hat{r} && \text{Spherical} \end{aligned}$$

This allows us to write the dot product using coordinates. If we write

$$\begin{aligned} \vec{A} &= A_x \hat{i} + A_y \hat{j} + A_z \hat{k} \\ \vec{B} &= B_x \hat{i} + B_y \hat{j} + B_z \hat{k} \end{aligned}$$

and multiply out $\vec{A} \cdot \vec{B}$, then we get

$$\begin{aligned} \vec{A} \cdot \vec{B} &= A_x B_x \hat{i} \cdot \hat{i} + A_x B_y \hat{i} \cdot \hat{j} + A_x B_z \hat{i} \cdot \hat{k} \\ &\quad + A_y B_x \hat{j} \cdot \hat{i} + A_y B_y \hat{j} \cdot \hat{j} + A_y B_z \hat{j} \cdot \hat{k} \\ &\quad + A_z B_x \hat{k} \cdot \hat{i} + A_z B_y \hat{k} \cdot \hat{j} + A_z B_z \hat{k} \cdot \hat{k} \\ &= A_x B_x + A_y B_y + A_z B_z \end{aligned} \tag{4.5}$$

It is rather remarkable that a rotation of the axes, as described in Section 4.1.1, has to give the same value in terms of the "primed" components. In fact, we formulate rotations mathematically by insisting that the dot product be *invariant* under a rotation transformation.

Another geometric vector product is the *cross product* $\vec{A} \times \vec{B}$, also depicted in Figure 4.1. Unlike the dot product, which is a (real) number, the cross product is itself another vector. The magnitude of $\vec{C} = \vec{A} \times \vec{B}$ is the area of the parallelogram formed by $\vec{A}$ and $\vec{B}$. Obviously, this means that the cross product of a vector with itself is zero, that is $\vec{A} \times \vec{A} = 0$.

The direction of the cross product usually makes use of something called the "right hand rule" which has had Physics students playing with their fingers for decades. I will be more precise about this shortly when we discuss cross product of unit vectors, but there is an easy way to visualize the direction of the cross product from Figure 4.1. Imagine that you are "turning" the direction of $\vec{A}$ into the direction $\vec{B}$, about an axis that is perpendicular to both of them.

Now imagine that you turning a typical screw in that direction. The direction that the screw advances is the direction of $\vec{C} = \vec{A} \times \vec{B}$. (The "typical" screw is right handed.) Of course, this means that $\vec{B} \times \vec{A} = -\vec{C}$.

Now consider the Cartesian unit vectors $\hat{i}$, $\hat{j}$, and $\hat{k}$. They are orthogonal, so the magnitude of their cross products is just unity. How we define the direction of their cross products, though, will set the "handedness" of the coordinate system. The convention that everyone sticks with, defining a "right handed" coordinate system, is the following:

$$\hat{i} \times \hat{j} = \hat{k} \tag{4.6a}$$
$$\hat{k} \times \hat{i} = \hat{j} \tag{4.6b}$$
$$\hat{j} \times \hat{k} = \hat{i} \tag{4.6c}$$

Notice how the vectors "cyclically rotate" through the three equations. If we reverse any one (or all three) of these definitions, the coordinate system would be "left handed."

The cross products of the unit vectors let us write out the cross product in terms of components, similar to the way we did it for the dot product. We have

$$\begin{aligned} \vec{A} \times \vec{B} &= A_x B_x \hat{i} \times \hat{i} + A_x B_y \hat{i} \times \hat{j} + A_x B_z \hat{i} \times \hat{k} \\ &\quad + A_y B_x \hat{j} \times \hat{i} + A_y B_y \hat{j} \times \hat{j} + A_y B_z \hat{j} \times \hat{k} \\ &\quad + A_z B_x \hat{k} \times \hat{i} + A_z B_y \hat{k} \times \hat{j} + A_z B_z \hat{k} \times \hat{k} \\ &= (A_y B_z - A_z B_y)\hat{i} + (A_z B_x - A_x B_z)\hat{j} + (A_x B_y - A_y B_x)\hat{k} \end{aligned} \tag{4.7}$$

Calculations with components using δ_{ij} and ϵ_{ijk}

Physics problems will often make use of dot products and cross products of both vector fields and vector derivatives (Section 4.2). We want to be efficient about these kinds of calculations, and there are some good tools for this. The first thing we want to do is associate and index $i = 1, 2, 3$ with components x, y, z. That is, we can rewrite the dot product from (4.5) as

$$\vec{A} \cdot \vec{B} = \sum_{i=1}^{3} A_i B_i$$

You can see that this is going to write a lot of summation signs, so we will implement the *summation convention* which says that if an index is repeated in an expression, it is implied

that we need to sum over that index, setting it equal to 1, 2, and 3, and adding up the terms. Therefore, we write

$$\vec{A} \cdot \vec{B} = A_i B_i$$

where the sum over i is implied. We will never allow ourselves to be in a situation where we need to sum over an index that appears more than twice. In fact, no expression should ever be written down where any index appears three times or more.

For the unit vectors we can write $\hat{e}_1 \equiv \hat{i}$, $\hat{e}_2 \equiv \hat{j}$, $\hat{e}_3 \equiv \hat{k}$,so

$$\vec{A} = A_i \hat{e}_i$$

is a handy way to write a vector. A second vector might be $\vec{B} = B_j \hat{e}_j$, where a different summation index j is used instead of i. In this case the dot product would be written

$$\vec{A} \cdot \vec{B} = A_i \hat{e}_i \cdot B_j \hat{e}_j = A_i B_j \, \hat{e}_i \cdot \hat{e}_j$$

where now this represents nine terms, summing over both i and j. Of course $\hat{e}_i \cdot \hat{e}_j$ equals unity if $i = j$ and is zero otherwise, so the nine terms collapse to the three terms represented by $A_i B_i$. There is a very convenient way to write this using the *Kronecker delta* δ_{ij}, defined simply as

$$\begin{aligned} \delta_{ij} &= 1 \quad \text{for} \quad i = j \\ &= 0 \quad \text{for} \quad i \neq j \end{aligned}$$

That is $\hat{e}_i \cdot \hat{e}_j = \delta_{ij}$ and we write

$$\vec{A} \cdot \vec{B} = A_i B_j \, \delta_{ij} = A_i B_i$$

The Kronecker delta effectively lets you "get rid of an index" in the implied sum.

There is a similar symbol that helps us work with cross products. I think it is more or less officially called the *Levi-Civita symbol for three dimensions*, most people I know refer to it as the *totally antisymmetric symbol.* We write it as ϵ with three indices that I'll call i, j, and k (not to be confused with the names of the unit vectors!) The definition is

$$\begin{aligned} \epsilon_{123} &= +1 \\ \text{and} \quad \epsilon_{ijk} &= -\epsilon_{jik} = -\epsilon_{ikj} - \epsilon_{kji} \end{aligned}$$

In other words, $\epsilon_{ijk} = 1$ if the i, j, k are in standard right-handed order, and flipping any two indices reverses the sign. Clearly, then, if any two indices are the same, then $\epsilon_{ijk} = 0$. We can then write the cross product $\vec{A} \times \vec{B}$ as

$$\vec{A} \times \vec{B} = \epsilon_{ijk} \hat{e}_i A_j B_k$$

a sum which, technically, has 9 terms, three of which are zero. We can also write

$$(\vec{A} \times \vec{B})_i = \epsilon_{ijk} A_j B_k$$

which gives the ith component of $\vec{A} \times \vec{B}$.

A very useful theorem which connects the totally antisymmetric symbol with the Kronecker delta, written using our summation convention, is

$$\epsilon_{ijk}\epsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km} \tag{4.8}$$

Note that the left side sums over i. I'm not going to bother trying to prove this, but if you want to write out some or all of the 81 equations represented here, that's up to you. Let's use this to prove something we generally call the "back-cab" rule, namely

$$\vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}(\vec{A} \cdot \vec{C}) - \vec{C}(\vec{A} \cdot \vec{B})$$

If we write this out for the ith component of the triple cross product, we get

$$\begin{aligned} \Big[\vec{A} \times (\vec{B} \times \vec{C})\Big]_i &= \epsilon_{ijk}A_j(\vec{B} \times \vec{C})_k = \epsilon_{ijk}A_j\epsilon_{kmn}B_mC_n = \epsilon_{kij}\epsilon_{kmn}A_jB_mC_n \\ &= (\delta_{im}\delta_{jn} - \delta_{in}\delta_{jm})A_jB_mC_n = A_jB_iC_j - A_jB_jC_i \\ &= B_i(\vec{A} \cdot \vec{C}) - C_i(\vec{A} \cdot \vec{B}) \end{aligned}$$

which is the "back-cab" rule for the ith component of $\vec{A} \times (\vec{B} \times \vec{C})$. Notice that I used a cyclic permutation (or, if you prefer, two index flips) to turn ϵ_{ijk} into ϵ_{kij} so that I could use (4.8), albeit with different index notation.

4.1.3 Plane polar, cylindrical, and spherical coordinates

Figure 1.3 shows how to locate a point in a plane using either Cartesian coordinates (x, y) or *plane polar* coordinates (r, ϕ). and how to locate a point in three dimensional space either Cartesian coordinates (x, y, z) or *spherical polar* coordinates (r, θ, ϕ). There is a second way to locate a point in three dimensional space, where plane polar coordinates are used in the xy plane, but the z-coordinate is intact. These are called *cylindrical polar* coordinates.

We can of course represent vectors in polar coordinates just as well as in Cartesian coordinates. It's the same vector! We are just using a different coordinate system to specify it. We would write[1]

$$\vec{A} = A_r\hat{r} + A_\phi\hat{\phi} + A_z\hat{k}$$

in cylindrical coordinates, and

$$\vec{A} = A_r\hat{r} + A_\theta\hat{\theta} + A_\phi\hat{\phi}$$

in spherical coordinates. The unit vectors have the same meaning as in the Cartesian case, *but these unit vectors have a direction that depends on the position of the point in space*

[1]Many texts will use ρ instead of r for the radial coordinate in cylindrical coordinates. I prefer to use r for either case, which makes sense for plane polar coordinates, and not switch when adding the z-coordinate in three dimensions.

to which they refer. This makes a huge difference if we ever need to calculate something like $\partial\vec{A}/\partial x$, since we need to consider the derivatives of the components *as well as the unit vectors.* Let's see how this works.

Let's start with plane polar coordinates. Figure 1.3 makes it clear that

$$x = r\cos\phi \tag{4.9a}$$
$$y = r\sin\phi \tag{4.9b}$$

Now imagine that we change the position $\vec{r}$ a tiny bit $d\vec{r} = dx\,\hat{i} + dy\,\hat{j}$. This means that x and y change by the infinitesimal amounts

$$\begin{aligned} dx &= \cos\phi\,dr - r\sin\phi\,d\phi \\ dy &= \sin\phi\,dr + r\cos\phi\,d\phi \end{aligned}$$

To find the unit vectors $\hat{r}$ ad $\hat{\phi}$, we consider the change $d\vec{r}$ happening in those two specific directions. To see what happens in the r-direction, set $d\phi = 0$. This gives

$$d\vec{r} = \hat{i}\cos\phi\,dr + \hat{j}\sin\phi\,dr = (\hat{i}\cos\phi + \hat{j}\sin\phi)dr = \hat{r}\,dr$$

where $\hat{r} = (\hat{i}\cos\phi + \hat{j}\sin\phi$ because it is clear that dr is the magnitude of $d\vec{r}$ when the change only happens in the r-direction. If instead we move in the ϕ-direction and set $dr = 0$, we get

$$d\vec{r} = -\hat{i}\,r\sin\phi\,d\phi + \hat{j}\,r\cos\phi\,d\phi = (-\hat{i}\sin\phi + \hat{j}\cos\phi)rd\phi = \hat{\phi}\,rd\phi$$

where $\hat{\phi} = -\hat{i}\sin\phi + \hat{j}\cos\phi$ because the distance along an arc at radius r through an angle $d\phi$ is $rd\phi$, and that is the change in the vector $\vec{r}$ when we move only in the ϕ-direction.

To summarize, then, the unit vectors for plane polar coordinates r and ϕ are

$$\hat{r} = \hat{i}\cos\phi + \hat{j}\sin\phi \tag{4.10a}$$
$$\hat{\phi} = -\hat{i}\sin\phi + \hat{j}\cos\phi \tag{4.10b}$$

The position vector is

$$\vec{r} = \hat{i}\;x + \hat{j}y = r(\hat{i}\cos\phi + \hat{j}\sin\phi) = r\hat{r} \tag{4.11}$$

and an infinitesimal change in the position vector is

$$d\vec{r} = \hat{i}\,dx + \hat{j}\,dy = dr\,\hat{r} + rd\phi\,\hat{\phi} \tag{4.12}$$

Figure 4.2 shows the unit vector orientations for both Cartesian and plane polar coordinates. *Unlike the Cartesian unit vectors $\hat{i}$ and $\hat{j}$, the unit vectors $\hat{r}$ and $\hat{\phi}$ change their direction as you move around the plane.* This will become a very important fact when it comes time to talk about derivatives in plane polar coordinates!

For cylindrical coordinates in three dimensions, we simply include the unit vector $\hat{k}$ in the z-direction. This is the same unit vector and coordinate as in the Cartesian system.

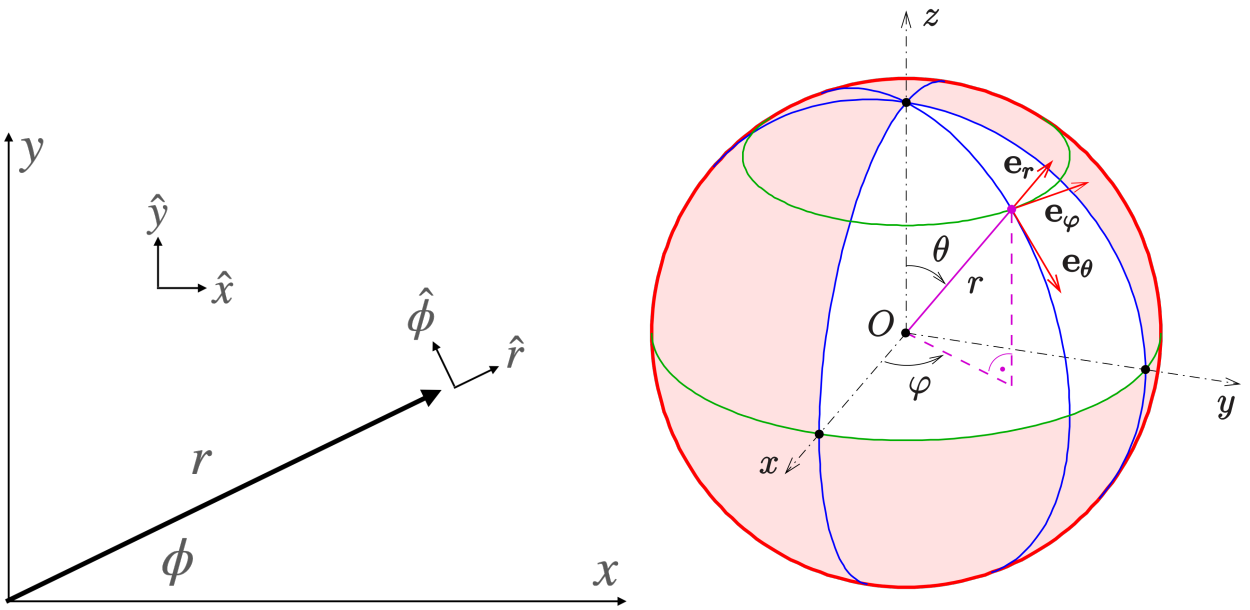


Figure 4.2: Unit vectors in the plane for Cartesian (x, y) coordinates and plane polar (r, ϕ) coordinates, and in three-dimensional space for spherical polar coordinates. It is important to note that while Cartesian unit vectors do not change their direction anywhere in the plane, the polar unit vectors indeed depend on r, θ, and ϕ. The spherical coordinates figure is taken from "By Ag2gaeh - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=43953509", and uses $\mathbf{e}_r$, $\mathbf{e}_\theta$, and $\mathbf{e}_\phi$ to denote the unit vectors, instead of $\hat{r}$, $\hat{\theta}$, and $\hat{\phi}$.

The situation is very similar for spherical polar coordinates. Figure 1.3 shows that the projection of the radial coordinate onto the xy plane is $r \sin\theta$. The transformation equations are therefore

$$x = r\sin\theta\cos\phi \tag{4.13a}$$
$$y = r\sin\theta\sin\phi \tag{4.13b}$$
$$z = r\cos\theta \tag{4.13c}$$

which leads to the spherical unit vectors in terms of the Cartesian unit vectors as

$$\hat{r} = \hat{\imath}\sin\theta\cos\phi + \hat{\jmath}\sin\theta\sin\phi + \hat{k}\cos\theta \tag{4.14a}$$
$$\hat{\theta} = \hat{\imath}\cos\theta\cos\phi + \hat{\jmath}\cos\theta\sin\phi - \hat{k}\sin\theta \tag{4.14b}$$
$$\hat{\phi} = -\hat{\imath}\sin\phi + \hat{\jmath}\cos\phi \tag{4.14c}$$

Plane polar coordinates and unit vectors can now be written directly from the spherical case for $\theta = \pi/2$. Figure 4.2 also depicts the spherical unit vectors.

4.1.4 Vector generalizations

When we get to Chapter 6 and Section 6.2, we will talk about the generalization of vectors to include *vector spaces*. Manipulating these generalized vectors will involve matrices and matrix operations, and will have very many applications to problems in the physical sciences.

Nevertheless, I want to mention here some generalizations that still maintain the ideas of vectors in physical space. Probably the first one that comes to mind is a concept you may encounter when studying Special Relatively, namely that "time is the fourth dimension." Indeed, the "three-vectors" we have been discussing here become "four-vectors" when including time as a dimension. We call this four-dimensional space *spacetime*. In this case, the vectors have four elements, with the time-like element having the index zero. A convention is that we use latin indices like i, j, and k when we run over the three spacial dimensions, and Greek indices like μ, ν, and σ when we run over 0, 1, 2, and 3.

We can denote the four-vectors of spacetime as $\mathsf{A} = (A_0, A_1, A_2, A_3) = (A_0, \vec{A})$. The most important difference when moving from vectors in space to spacetime is in the dot product. In this case, the dot product must be invariant under Lorentz Transformation, which implies that the dot product between two four-vectors A and B becomes

$$\mathsf{A} \cdot \mathsf{B} = A_0 B_0 - A_1 B_1 - A_2 B_2 - A_3 B_3 = A_0 B_0 - \vec{A} \cdot \vec{B}$$

where the relative minus sign between the spacelike and timelike components has many physical implications.

A more general application of spacetime, which is necessary for understanding General Relativity and the theory of gravitation, comes from the need to recognize that there are in fact two different geometric classes of spatial vectors. These are called *contravariant vectors* and *covariant vectors*, aka "vectors" and "covectors." We are not going to discuss these further in this course, but if you want to read a little bit about them, see "Answer to Question #55. Are there pictorial examples that distinguish covariant and contravariant vectors?", American Journal of Physics 65, 1037 (1997) by J. Napolitano and R. Lichtenstein, https://doi.org/10.1119/1.18743.

4.2 Vector operators

Now we turn our attention to *spatial differential vector operators*. These are constructs that take (partial) derivatives of functions of spatial position, i.e. *fields*. We will construct these operators first in Cartesian coordinates, but then also give them, with some derivations, in cylindrical and spherical coordinates.

Most of the material in this section should be review, from either your Calculus classes or your Wave Physics class.

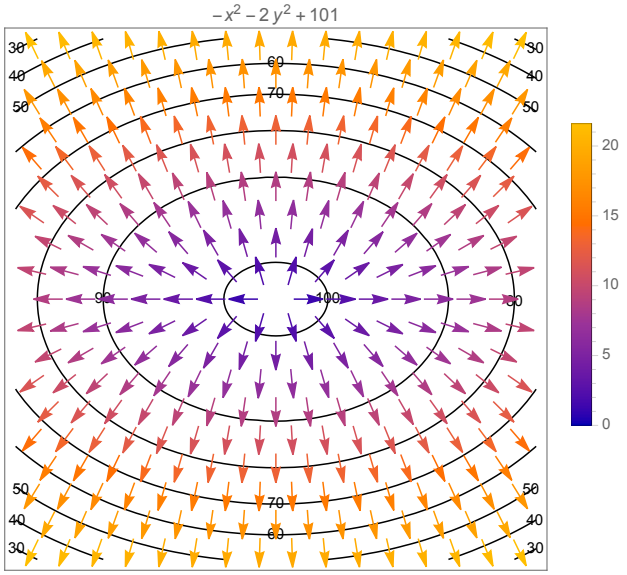


Figure 4.3: Visualizating the gradient of $f(\vec{r}) = f(x, y) = 101 - x^2 - 2y^2$, a scalar field in two spatial dimensions. The function $f(x, y)$ is drawn as a contour plot, with the contours labeled. The (negative of its) gradient $-\vec{\nabla} f = 2x\hat{i} + 4y\hat{j}$ is drawn with arrows at different points (x, y) that point in the direction of the gradient, and whose color indicates the magnitude $|\vec{\nabla} f|$ at that point. Notice that the magnitude of the gradient is larger in the regions where the contours are more steep. (I plot $-\vec{\nabla} f$ instead of $\vec{\nabla} f$ because it feels better to go down the hill instead of up it.)

4.2.1 Gradient

Suppose you have a scalar field $f(\vec{r}) = f(x, y, z)$ (or $f(x, y)$ in two dimensions) over some region in space. You will typically need to know how fast that function changes, that is, you will need to know its derivative. However, the rate of change will depend on which direction in space you are moving. Somehow we need to come up with a "derivative" that respects the direction in space. In other words, we need a vector version of the derivative.

That vector version of the derivative is called the *gradient* of $f(\mathbf{r})$, written in Cartesian coordinates as

$$\vec{\nabla} f = \hat{i}\frac{\partial f}{\partial x} + \hat{j}\frac{\partial f}{\partial y} + \hat{k}\frac{\partial f}{\partial z}$$

This vector quantity, in principle different at any different point in space, will tell the direction in which the change of $f(\mathbf{r})$ is a maximum. Figure 4.3 is a visualization of the gradient for a particular two-dimensional scalar field. (Actually, it is the negative of the gradient that is plotted, only because it feels more natural to go down the hill instead of up it.) Notice how the magnitude of the gradient (given by the color of the arrow) is larger where the hill is steeper.

It is not hard to see that the gradient tells us the direction in which the change is $f(\vec{r})$ is greatest. Consider moving in some direction $\vec{s}$. The infinitesimal change in the distance along $\vec{s}$ is ds, so the derivative of $f(\vec{r})$ in this direction is

$$\frac{df}{ds} = \frac{1}{ds}df = \frac{1}{ds}\left[\frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz\right] = \vec{\nabla} f \cdot \left[\hat{i}\frac{dx}{ds} + \hat{j}\frac{dy}{ds} + \hat{k}\frac{dz}{ds}\right] = \vec{\nabla} f \cdot \hat{s}$$

where $\hat{s}$ is the unit vector in the s-direction, since $ds^2 = dx^2 + dy^2 + dz^2$. Of course, $\vec{\nabla} f \cdot \hat{s} = |\vec{\nabla} f| \cos\psi$ where ψ is the angle between the gradient and $\vec{s}$. Therefore, the direction of greatest change is when $\psi = 0$, that is, in the direction of the gradient.

We will find it handier to think of $\vec{\nabla}$ as a *vector operator* which we write as

$$\vec{\nabla} = \hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z} \qquad \text{Cartesian coordinates} \tag{4.15}$$

In other words, $\vec{\nabla} f$ is the gradient operator "acting on" the field $f(\vec{r})$. Similarly, we can think of $\hat{i} \cdot \vec{\nabla} f = \partial/\partial x$ as a differential operator, and so forth.

It is straightforward to write down the gradient operator in different coordinate systems. For example, if $f(\vec{r})$ is expressed in cylindrical coordinates r, ϕ, z, then

$$\vec{\nabla} f = \hat{i}\frac{\partial f(r,\phi,z)}{\partial x} + \hat{j}\frac{\partial f(r,\phi,z)}{\partial y} + \hat{k}\frac{\partial f(r,\phi,z)}{\partial z}$$

and we use the chain rule to express the derivatives in terms of r, ϕ, z. We have

$$\frac{\partial f}{\partial x} \;=\; \frac{\partial f}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x} + \frac{\partial f}{\partial z}\frac{\partial z}{\partial x}$$

Inverting (4.9) gives

$$r = \left(x^2 + y^2\right)^{1/2} \qquad \text{so} \qquad \frac{\partial r}{\partial x} = \frac{x}{(x^2+y^2)^{1/2}} = \frac{x}{r} = \cos\phi$$

and

$$\tan\phi = \frac{y}{x} \qquad \text{so} \qquad \frac{1}{\cos^2\phi}\frac{\partial \phi}{\partial x} = -\frac{y}{x^2} = \frac{-r\sin\phi}{r^2\cos^2\phi} \qquad \text{and} \qquad \frac{\partial \phi}{\partial x} = -\frac{1}{r}\sin\phi$$

Of course, $\partial z/\partial x = 0$ so the first term of $\vec{\nabla} f$ in cylindrical coordinates is

$$\hat{i}\frac{\partial f(r,\phi,z)}{\partial x} = \hat{i}\left[\frac{\partial f}{\partial r}\cos\phi + \frac{1}{r}\frac{\partial f}{\partial \phi}(-\sin\phi) + 0\right] = \hat{i}\left[\cos\phi\frac{\partial f}{\partial r} - \sin\phi\frac{1}{r}\frac{\partial f}{\partial \phi}\right]$$

(Note the $1/r$ factor in front of the ϕ derivatives, which makes the expression dimensionally correct.) Similarly, the second term is

$$\hat{j}\frac{\partial f(r,\phi,z)}{\partial y} = \hat{j}\left[\sin\phi\frac{\partial f}{\partial r} + \cos\phi\frac{1}{r}\frac{\partial f}{\partial \phi}\right]$$

The third term is just $\hat{k}\partial f/\partial z$, or simply missing if we are working in plane polar coordinates. Putting this all together, the gradient becomes

$$\begin{aligned}
\vec{\nabla} f &= \hat{i}\left[\cos\phi\frac{\partial f}{\partial r} - \sin\phi\frac{1}{r}\frac{\partial f}{\partial \phi}\right] + \hat{j}\left[\sin\phi\frac{\partial f}{\partial r} + \cos\phi\frac{1}{r}\frac{\partial f}{\partial \phi}\right] + \hat{k}\frac{\partial f}{\partial z} \\
&= (\hat{i}\cos\phi + \hat{j}\sin\phi)\frac{\partial f}{\partial r} + (-\hat{i}\sin\phi + \hat{j}\cos\phi)\frac{1}{r}\frac{\partial f}{\partial \phi} + \hat{k}\frac{\partial f}{\partial z} \\
&= \hat{r}\frac{\partial f}{\partial r} + \hat{\phi}\frac{1}{r}\frac{\partial f}{\partial \phi} + \hat{k}\frac{\partial f}{\partial z}
\end{aligned}$$

where we made use of the expressions (4.10) for the unit vectors in plane polar coordinates. This means that the gradient operator in cylindrical coordinates is

$$\vec{\nabla} = \hat{r}\frac{\partial}{\partial r} + \hat{\phi}\frac{1}{r}\frac{\partial}{\partial \phi} + \hat{k}\frac{\partial}{\partial z} \qquad \text{Cylindrical coordiantes} \tag{4.16}$$

It's nice to see this carried out from the fundamentals, but there is in fact an easier way to get this result. In plane polar coordinates, the infinitesimal change in the position vector is given by (4.12). If you think of the gradient as the directional derivative, simple inspection shows that if you move in the radial direction only, the derivative is $\partial/\partial r$. On the other hand, if you move in the axial direction only, the derivative is $(1/r)\partial/\partial\phi$. Including the z-coordinate, then, the gradient operator is clearly (4.16).

For spherical coordinates, you carry through exactly the same way, but using (4.13) instead of (4.10). You find

$$\vec{\nabla} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi} \qquad \text{Spherical coordiantes} \tag{4.17}$$

I'll leave deriving this as a homework problem.

4.2.2 Divergence

We can define other operators based on the gradient operator. Given a vector field

$$\vec{V}(\vec{r}) = \vec{V}(x,y,z) = \hat{i}V_x(x,y,z) + \hat{j}V_y(x,y,z) + \hat{k}V_z(x,y,z) \tag{4.18}$$

we can use the gradient operator to measure how much the field "diverges" in a region of space. I'll make clearer what I mean by that in Section 4.3.2, but for now just think of it measuring how much of $\vec{V}(\vec{r})$ has a "flow" that emerges from a region of space.

We define the *divergence* of a vector field $\vec{V}(\vec{r}) = \vec{V}(x,y,z)$ as

$$\vec{\nabla}\cdot\vec{V} = \frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial z} \tag{4.19}$$

where we are literally taking the dot product of the vector operator $\vec{\nabla}$ with the vector field $\vec{V}$. It is very important to note that when we did this, we treated the unit vectors $\hat{i}$, $\hat{j}$, and $\hat{k}$ as constants. Indeed, they do not depend on position. However, this will not be the case when we consider cylindrical and spherical coordinates.

I'm not going to bother deriving the form of the gradient in cylindrical or spherical coordinates, nor will I assign them as homework. They are tedious calculations, and not, in my opinion, particularly instructive, although it is good practice in partial derivatives and the chain rule to carry through the calculation. Instead, I will just state the results, which you

can find many places online or in textbooks. We find

$$\vec{\nabla}\cdot\vec{V} = \frac{1}{r}\frac{\partial}{\partial r}(rV_r) + \frac{1}{r}\frac{\partial V_\phi}{\partial\phi} + \frac{\partial V_z}{\partial z} \qquad \text{Cylindrical} \tag{4.20}$$

$$\vec{\nabla}\cdot\vec{V} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2V_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\, V_\theta) + \frac{1}{r\sin\theta}\frac{\partial V_\phi}{\partial\phi} \qquad \text{Spherical} \tag{4.21}$$

4.2.3 Curl

Applying the cross product of the gradient operator to a vector field is called the *curl*, for reasons that will become apparent in Section 4.3.1. We have

$$\vec{\nabla}\times\vec{V} = \hat{i}\left(\frac{\partial V_z}{\partial y} - \frac{\partial V_y}{\partial z}\right) + \hat{j}\left(\frac{\partial V_x}{\partial z} - \frac{\partial V_z}{\partial x}\right) + \hat{k}\left(\frac{\partial V_y}{\partial x} - \frac{\partial V_x}{\partial y}\right) \tag{4.22}$$

$$\vec{\nabla}\times\vec{V} = \hat{r}\left(\frac{1}{r}\frac{\partial V_z}{\partial\phi} - \frac{\partial V_\phi}{\partial z}\right) + \hat{\phi}\left(\frac{\partial V_r}{\partial z} - \frac{\partial V_z}{\partial r}\right) + \hat{k}\frac{1}{r}\left(\frac{\partial}{\partial r}rV_\phi - \frac{\partial V_r}{\partial\phi}\right) \tag{4.23}$$

$$\begin{aligned}\vec{\nabla}\times\vec{V} = {} & \hat{r}\frac{1}{r\sin\theta}\left(\frac{\partial}{\partial\theta}V_\phi\sin\theta - \frac{\partial V_\theta}{\partial\phi}\right) + \hat{\theta}\frac{1}{r}\left(\frac{1}{\sin\theta}\frac{\partial V_r}{\partial\phi} - \frac{\partial}{\partial r}rV_\phi\right) \\ & + \hat{\phi}\frac{1}{r}\left(\frac{\partial}{\partial r}rV_\theta - \frac{\partial V_r}{\partial\theta}\right)\end{aligned} \tag{4.24}$$

in Cartesian, cylindrical polar, and spherical polar coordinates, respectively.

Although it may be more or less obvious from general ideas about vector cross products and dot products, it is worth stating outright that (1) the curl of any gradient is zero, and (2) the divergence of any curl is zero. That is

$$\vec{\nabla}\times\vec{\nabla}f(\vec{r}) = 0$$

for any scalar field $f(\vec{r})$, and

$$\vec{\nabla}\cdot\left[\vec{\nabla}\times\vec{V}(\vec{r})\right] = 0$$

for any vector field $\vec{V}(\vec{r})$. You will see in your electromagnetism classes that this is the basis for defining the scalar and vector potentials.

4.2.4 The Laplacian

You will encounter many calculations in Physics where you want to take the divergence of some vector field, which itself is the gradient of some scalar field.[2] This leads to the (scalar)

[2]Probably the first example of this is taking the divergence of the electric field, written as the (negative) gradient of the electric potential.

operator $\vec{\nabla}^2 = \vec{\nabla} \cdot \vec{\nabla}$ known as the *Laplacian*. Its form in Cartesian coordinates is obvious, namely

$$\vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{4.25}$$

The form of the Laplacian in cylindrical or spherical coordinates is less obvious, but straightforward to derive. As always, you need to remember that that unit vectors in this case need to be differentiated because they depend on position. One finds

$$\vec{\nabla}^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \qquad \text{Cylindrical} \tag{4.26}$$

$$\vec{\nabla}^2 = \frac{1}{r^2}\frac{\partial}{\partial r^2}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2} \qquad \text{Spherical} \tag{4.27}$$

You will find in Section 4.5.1 that the radial part of (4.26) gives rise to Bessel's Equation (3.19), the radial part of (4.27) leads to spherical Bessel functions, and the θ equation from (4.27) becomes Legendre's Equation (3.29).

It should be clear that you can apply the Laplacian operator to either a scalar field or a vector field. In case of the latter, you just need to apply it to each component, which can be tricky if you are applying the operator in cylindrical or spherical coordinates to a vector field in cylindrical or spherical coordinates. In general, we try to avoid having to deal with such situations!

4.3 Surface Theorems

Probably the most important physical applications of vector calculus have to do with a class of properties that I'll call *surface theorems*. We will discuss two of these in particular, namely Stokes' Theorem and Gauss' Theorem. (I think mathematicians probably refer to Gauss' Theorem as the Divergence Theorem.)

The idea behind the surface theorems is that whatever is going on inside some closed region can be inferred from what is happening on the surface of that region. Stokes' Theorem applies to regions enclosed by a loop in space, and Gauss' Theorem applies to volumes and the surfaces that enclose them.

This section will first state and then prove Stokes' Theorem first, then Gauss' Theorem. These two theorems are intimately connected to the curl and divergence, respectively, of a vector field. In fact, a better way to present the curl and divergence would be to see how they arise naturally from these theorems. This is the approach taken in a popular text from many years ago, called "Div, Grad, Curl, and All That: An Informal Text on Vector Calculus", bu H.M. Schey. It's a nice book, and it shouldn't be too hard for you to locate a copy if you would like to look it over.

4.3.1 Stokes' theorem

Stokes' Theorem relates the integral of some vector quantity projected onto a closed loop, to the curl of that vector field integrated over the surface enclosed by the loop. We state this theorem mathematically as

$$\oint_C \vec{A} \cdot d\vec{\ell} = \int_S (\vec{\nabla} \times \vec{A}) \cdot d\vec{S} \tag{4.28}$$

where C is the closed loop and S is the surface that it encloses. The shape of the surface doesn't matter, just so long as its edges lie along C. The integrand $\vec{A} \cdot d\vec{\ell}$ means the dot product of the vector field with a tiny line segment pointing along the line, and the little circle on the integral sign just means the line forms a closed loop. On the right hand integral, the vector $d\vec{S}$ is an infinitesimal whose magnitude dS is the size of the area element of S, and the direction is normal to the surface. The sign of the normal is determined by an agreement of using the right hand rule based on an assigned direction for following the loop.

We can prove Stokes' Theorem by first taking the surface S and carving it up into a bunch of tiny rectangles. We'll assume that S lies in the xy plane, and argue later that we can generalize to any curve. Each tiny rectangle has width dx and height dy. We'll then show that Stokes' Theorem holds for each tiny rectangle by itself.

Now if I put two tiny rectangles next to each other, then the line integral on the left side of (4.28) cancels along the adjacent edge, and the curve is over the pair of rectangles. Keep going, and eventually you'll cover the entire surface S, and the only curve that's left is C. At this point, we can say that we've proved Stokes' Theorem.

Figure 4.4 shows how this works. The sum of $\vec{A} \cdot d\vec{\ell}$ over the tiny square's sides is

$$\begin{aligned} \sum \vec{A} \cdot d\vec{\ell} &= A_x(x,y)dx + A_y(x+dx,y)dy - A_x(x+dx,y+dy)dx - A_y(x,y+dy)dy \\ &= [A_x(x,y) - A_x(x+dx,y+dy)]dx + [A_y(x+dx,y) - A_y(x,y+dy)]dy \end{aligned}$$

where we note that, for example, $\vec{A} \cdot d\vec{\ell} = A_x\, dx$ when $d\vec{\ell}$ is in the x-direction, and so forth. Care is taken to evaluate the components of the vector function consistently at the corner of the rectangle where piece of the integral starts. Now factoring out $dx\, dy$ and doing some rearranging, we get

$$\sum \vec{A} \cdot d\vec{\ell} = \left[\frac{A_y(x+dx,y) - A_y(x,y+dy)}{dx} - \frac{A_x(x+dx,y+dy) - A_x(x,y)}{dy} \right] dx\, dy$$

As the infinitesimals approach zero, the two expressions in the brackets become partial derivatives. The result is

$$\sum \vec{A} \cdot d\vec{\ell} = \left[\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right] dx\, dy = (\vec{\nabla} \times \vec{A})_z\, dx\, dy$$

where, finally, we recognize that combination of partial derivatives as the z-component of the curl. Since $dx\, dy = dS$ and, in this case, the normal to the surface is $\hat{z}$, we have, for the

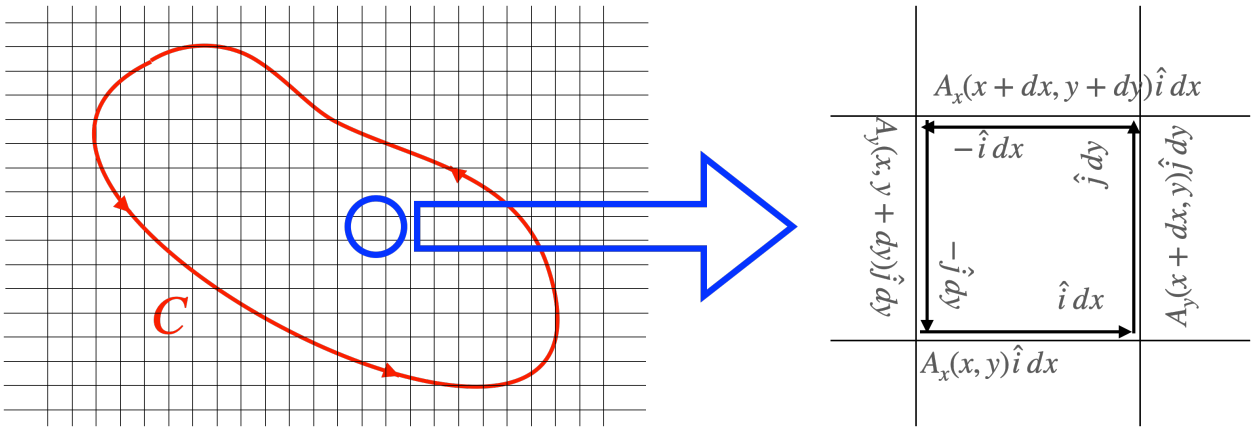


Figure 4.4: Figure used in the proof of Stokes' Theorem. An arbitrary curve C bounds some surface S, which in this example lies in the xy plane. The plane is divided up into a bunch of infinitesimal rectangles with dimension $dx \times dy$. The dot product $\vec{A} \cdot d\vec{\ell}$ is evaluated first along the sides of a tiny rectangle with lower left corner at the point (x, y). This is then generalized to include the entire curve C.

tiny rectangle,

$$\sum \vec{A} \cdot d\vec{\ell} = (\vec{\nabla} \times \vec{A}) \cdot d\vec{S}$$

Adding up all the little rectangles, and recognizing that their edges cancel in the line integral leaving only the curve C, we get (4.28).

I'll argue that the shape of the surface doesn't matter until after we've done Gauss' Theorem.

Let's illustrate this with a simple example. Take a vector field $\vec{A} = -y\hat{i} + x\hat{j}$, which clearly has a "curl" to it if you plot[3] it with MATHEMATICA. In fact

$$\vec{\nabla} \times A = \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \hat{k} = (1+1)\hat{k} = 2\hat{k}$$

Take the curve C to be the square in the xy plane with side length ℓ and the lower left corner at the origin. The surface S has area ℓ^2 so the right hand side of (4.28) is

$$\int (\vec{\nabla} \times \vec{A}) \cdot d\vec{S} = 2 \int dS = 2\ell^2$$

Now let's evaluate the line integral. Going counter clockwise from the lower left corner,

$$\begin{aligned} \oint \vec{A} \cdot d\vec{\ell} &= \int_{x=0}^{\ell} (-y)|_{y=0}\, dx + \int_{y=0}^{\ell} (x)|_{x=\ell}\, dy + \int_{x=\ell}^{0} (-y)|_{y=\ell}\, dx + \int_{y=\ell}^{0} (x)|_{x=0}\, dy \\ &= 0 + \ell \cdot \ell - \ell \cdot (-\ell) = 2\ell^2 \end{aligned}$$

as predicted by the theorem.

[3]This is simple to do. Just define v = {-y, x} and then enter VectorPlot[v, {x, -3, 3}, {y, -3, 3}].

Note that for this field, with a constant curl, it shouldn't matter where we put the square! We'll evaluate it for the example given, but you should try putting it somewhere else, perhaps centered on the origin, to confirm that you get the same answer.

4.3.2 Gauss' theorem

Gauss' Theorem (also known as the *Divergence Theorem*) relates the divergence of a vector field in some volume V to the surface integral of the normal component of the vector field over the surface S that encloses the volume. That is,

$$\oint_S \vec{A} \cdot d\vec{S} = \int_V \vec{\nabla} \cdot \vec{A}\, dV \tag{4.29}$$

When $\vec{A}$ is physically describing the "flow" of some quantity, in which case $\vec{A} \cdot d\vec{S}$ is the "flux" through the surface $d\vec{S}$, we will find this to be an extremely useful theorem.

The proof of Gauss' Theorem is very similar to how we proved Stokes' Theorem. In this case, you chop up the volume V into a bunch of tiny bricks, with dimensions dx, dy, and dz. For one of these tiny bricks, the surface integral is the sum

$$\begin{aligned}
\sum \vec{A} \cdot d\vec{S} &= A_x(x+dx,y,z)(+dy\,dz) + A_x(x,y,z)(-dy\,dz) \\
&+ A_y(x,y+dy,z)(+dx\,dz) + A_y(x,y,z)(-dx\,dz) \\
&+ A_z(x,y,z+dz)(+dx\,dy) + A_z(x,y,z)(-dx\,dy)
\end{aligned}$$

where I've paired the terms by the "front" and "back" of each of the three directions. Factoring out $dx\,dy\,dz = dV$, this expression becomes

$$\begin{aligned}
\sum \vec{A} \cdot d\vec{S} &= \left[\frac{A_x(x+dx,y,z) - A_x(x,y,z)}{dx} \right. \\
&\quad + \frac{A_y(x,y+dy,z) - A_y(x,y,z)}{dy} \\
&\quad \left. + \frac{A_z(x,y,z+dz) - A_z(x,y,z)}{dy} \right] dx\,dy\,dz \\
&= \left[\frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \right] dx\,dy\,dz = \vec{\nabla} \cdot \vec{A}\, dV
\end{aligned}$$

When we add up all of the little bricks, the right side just becomes the volume integral. On the left side, adjacent sides of bricks cancel $\vec{A} \cdot d\vec{S}$ because the vector $d\vec{S}$ has the same magnitude but opposite direction, and all that is left from the sum is the surface S that encloses the volume V. This proves (4.29).

Let's do a simple example with the field $\vec{A} = x\hat{i} + y\hat{j} + z\hat{k}$. This field clearly "diverges", as VectorPlot in MATHEMATICA will tell you. The divergence of this field is $\vec{\nabla} \cdot \vec{A} = 3$, that is, uniform everywhere, so the volume integral on the right side of (4.29) is just $3V$. A simple

shape is a cube of side length ℓ that sits in the first octant with a corner at the origin. The flux $\vec{A} \cdot d\vec{S}$ is zero on the three faces that are in the three planes $x = 0$, $y = 0$, and $z = 0$ because the component perpendicular to the plane is zero there. The flux on the other three faces is just $\ell \cdot \ell^2 = \ell^3$, so the surface integral is $3\ell^3 = 3V$. It works.

Why the surface shape doesn't matter in Stokes' Theorem

We gave a proof of (4.28) that assumed the surface was flat. Imagine there is now another surface that has the same curve C on the edge. These two surfaces form a closed volume, and the second surface has the opposite clockwise sense of the first. That is

$$\oint_{S_1+S_2} \vec{B} \cdot d\vec{S} = \int_{S_1} \vec{B} \cdot d\vec{S} - \int_{S_2} \vec{B} \cdot d\vec{S}$$

for some vector field $\vec{B}$. In the case of Stokes' Theorem, though, $\vec{B} = \vec{\nabla} \times \vec{A}$ for a different vector field $\vec{V}$. Now by Gauss' Theorem,

$$\oint_{S_1+S_2} \vec{B} \cdot d\vec{S} = \int_V \vec{\nabla} \cdot \vec{B} = \int_V \vec{\nabla} \cdot (\vec{\nabla} \times \vec{A}) = 0$$

since the divergence of any curl is zero. Therefore

$$\int_{S_1} \vec{B} \cdot d\vec{S} = \int_{S_2} \vec{B} \cdot d\vec{S}$$

so it doesn't matter which surface I use to be enclosed by C in Stokes' Theorem.

4.3.3 The continuity equation

The notion of a *conservation law* is fundamental in Physics. We say that quantities like charge, energy, and momentum, for example, are "conserved". That is, they do not change with time. How can we write this down, mathematically, for quantities that can exist spread out over space?

We will explore the answer to this question by considering three dimensional space. You can work the problem out for two dimensional space, in which case the answer will involve the curl. That might make a nice homework problem.

Imagine that we have some quantity Q that is spread over some volume V of space. We would write Q in terms of some scalar field $\rho(\vec{r}, t)$, namely the density of the material that makes up Q. The density has dimensions of $[Q]L^{-3}$, and it is possible that the density at any point can change with time t.

If Q is a conserved quantity, though, the only way it can change is if some of it flows into, our out of, the volume V. It is not possible to create or destroy the material that makes up Q if it is conserved. That is, there are no "sources" or "sinks" for this material inside V.

Define a vector field $\vec{j}(\vec{r},t)$ that represents the "flow" of this material. We'll write that the "flux" of this material through some area element $d\vec{S}$ is just $\vec{j}(\vec{r},t)\cdot d\vec{S}$. This makes sense because you recall that the direction of $d\vec{S}$ is perpendicular to the surface, so if the flow $\vec{j}(\vec{r},t)$ is perpendicular to the surface, then it is maximized, whereas it is zero if $\vec{j}(\vec{r},t)$ is parallel to the surface.

The dimensions of $\vec{j}(\vec{r},t)$ are $[Q]L^{-2}T^{-1}$ so the dimensions of the flux are $[Q]T^{-1}$. Sometimes we refer to $\vec{j}(\vec{r},t)$ as the "flux density," or "current density" particularly if Q represents electric charge.

Now consider the surface S that encloses the volume V. We know that the only way to change Q is for there to be some flux through S. Let's agree that a positive value for the flux is when the flow goes from the inside to the outside. This means that $\vec{j}(\vec{r},t)\cdot d\vec{S}$ is positive when $d\vec{S}$ is defined according to our normal convention that it points away from the inside of S. Integrating over the surface tells us how to write down the change of Q with time, namely

$$\frac{dQ}{dt} = -\oint_S \vec{j}(\vec{r},t)\cdot d\vec{S}$$

The minus sign tells us that if the net flux through the closed surface S is positive, then Q decreases, which is correct.

If we write Q in terms of the density $\rho(\vec{r},t)$ by integrating over the volume V, and we apply Gauss' Theorem to the surface integral, this equation becomes

$$\frac{d}{dt}\int_V \rho(\vec{r},t)\,dV = -\int_V \vec{\nabla}\cdot\vec{j}(\vec{r},t)\,dV$$

The time derivative is a total derivative because all that is left after doing the integral over position is time. I can bring the time derivative inside the integral, but then it becomes a partial derivative. this all leads us to

$$\int_V \left[\frac{\partial\rho(\vec{r},t)}{\partial t} + \vec{\nabla}\cdot\vec{j}(\vec{r},t)\right] dV = 0$$

Finally, we let the volume $V \to \Delta V$ be so small that we can neglect the change in the integrand over position and pull it out of the integral, leaving just the volume ΔV times the expression in square brackets, which itself now must be zero. Therefore

$$\frac{\partial\rho(\vec{r},t)}{\partial t} + \vec{\nabla}\cdot\vec{j}(\vec{r},t) = 0 \tag{4.30}$$

This differential equation is called the *Continuity Equation* and is the mathematical way to state that a quantity is conserved. It is used extensively in many fields of Physics, including fluid dynamics, electrodynamics, biological systems, statistical mechanics, and even finance.

4.3.4 Application to Maxwell's Equations

An important first application of the surface theorems is to turn Maxwell's Equations into their differential form. You likely learned the integral form of Maxwell's Equations in your introductory Physics class, namely[4]

$$\oint \vec{E} \cdot d\vec{S} = 4\pi Q_{\text{enclosed}} = 4\pi \int_V \rho \, dV \qquad \text{Gauss}' \text{ Law} \tag{4.31a}$$

$$\oint \vec{B} \cdot d\vec{S} = 0 \qquad \text{Gauss}' \text{ Law for Magnetism} \tag{4.31b}$$

$$\oint_C \vec{E} \cdot d\vec{\ell} = -\frac{1}{c}\frac{d\Phi_B}{dt} = -\frac{1}{c}\frac{d}{dt}\int_S \vec{B} \cdot d\vec{S} \qquad \text{Faraday}'\text{s Law} \tag{4.31c}$$

$$\begin{aligned} \oint_C \vec{B} \cdot d\vec{\ell} &= \frac{4\pi}{c} I_{\text{enclosed}} + \frac{1}{c}\frac{d\Phi_E}{dt} \\ &= \frac{4\pi}{c}\int_S \vec{j} \cdot d\vec{S} + \frac{1}{c}\frac{d}{dt}\int \vec{E} \cdot d\vec{S} \qquad \text{Ampere}'\text{s Law} \end{aligned} \tag{4.31d}$$

where I trust you remember terms like "Gaussian surface" and "Amperian loop."

Surface theorems can be used to turn each of the integrals on the left side into integrals over the Gaussian surface enclosing the volume, or Amperian loop enclosing the surface. For Gauss' Law, the charge enclosed by the Gaussian surface is just an integral over the volume of the charge density $\rho(\vec{r}, t)$. The current enclosed by the Amperian loop is just the current density $\vec{j}(\vec{r}, t)$ integrated over the surface it encloses. Therefore, these equations become

$$\vec{\nabla} \cdot \vec{E} = 4\pi\rho \qquad \text{Gauss}' \text{ Law} \tag{4.32a}$$

$$\vec{\nabla} \cdot \vec{B} = 0 \qquad \text{Gauss}' \text{ Law for Magnetism} \tag{4.32b}$$

$$\vec{\nabla} \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t} \qquad \text{Faraday}'\text{s Law} \tag{4.32c}$$

$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c}\vec{j} + \frac{1}{c}\frac{\partial \vec{E}}{\partial t} \qquad \text{Ampere}'\text{s Law} \tag{4.32d}$$

This form of Maxwell's equations is much more amenable to studying the properties of charges and currents than is the integral form. It will also allow us to see immediately how they predict the existence of electromagnetic waves, which we will discuss in Section 4.3.4, and that electric charge is conserved, which we'll investigate now.

Conservation of electric charge

It is easy to show that (4.32) imply that electric charge is conserved. That is, it is easy to show that they lead to the continuity equation for the electric charge density $\rho(\vec{r}, t)$ and

[4] I am writing these in Gaussian units, which are favored among physicists. Engineers typically use SI units, which is likely how you saw them in your first class.

current density $\vec{j}(\vec{r},t)$. First take the divergence of both sides of Ampere's Law. You know that the divergence of any curl is zero, so the left hand side must be zero. This gives us

$$0 = \frac{4\pi}{c}\vec{\nabla}\cdot\vec{j} + \frac{1}{c}\frac{\partial}{\partial t}\vec{\nabla}\cdot\vec{E}$$

Now use Gauss' Law to write $\vec{\nabla}\cdot\vec{E} = 4\pi\rho$. The overall factor of $4\pi/c$ cancels and you get

$$0 = \vec{\nabla}\cdot\vec{j} + \frac{\partial\rho}{\partial t}$$

which is just the continuity equation (4.30).

Maxwell's Equations imply that electric charge is conserved. This very important aspect of electrodynamics is often overlooked in classes on the subject.

Existence of electromagnetic waves

Maxwell's Equations predict the existence of electromagnetic waves. Mathematically, this means that Maxwell's Equations predict that there are forms of $\vec{E}(\vec{r},t)$ and $\vec{B}(\vec{r},t)$ that satisfy a partial differential equation known as the Wave Equation. We will look at how we go about solving this and similar equations in Sections 4.5 and 5.1, but for now, let's just go ahead and manipulate Maxwell's Equations to get the Wave Equation.

First, though, we will take a moment to prove a vector differential operator identity, namely

$$\vec{\nabla}\times(\vec{\nabla}\times\vec{A}) = \vec{\nabla}(\vec{\nabla}\cdot\vec{A}) - \vec{\nabla}^2\vec{A} \tag{4.33}$$

This is easy to do using the "δ,ϵ" technique of Section 4.1.2. Using the summation notation with our generic notation for Cartesian unit vectors, the gradient operator becomes

$$\vec{\nabla} = \hat{e}_i\frac{\partial}{\partial x_i}$$

where $x_1 = x$, $x_2 = y$, and $x_3 = z$. Since none of the $\hat{e}_i$ depend on position, we can just work with the components directly, and write

$$\begin{aligned}
[\vec{\nabla}\times(\vec{\nabla}\times\vec{A})]_i &= \epsilon_{ijk}\frac{\partial}{\partial x_j}\left(\epsilon_{kmn}\frac{\partial}{\partial x_m}A_n\right) = \epsilon_{kij}\epsilon_{kmn}\frac{\partial^2 A_n}{\partial x_j x_m} \\
&= (\delta_{im}\delta_{jn} - \delta_{in}\delta_{jm})\frac{\partial^2 A_n}{\partial x_j x_m} = \frac{\partial^2 A_j}{\partial x_j x_i} - \frac{\partial^2 A_i}{\partial x_j x_j} \\
&= \frac{\partial}{\partial x_i}\frac{\partial A_j}{\partial x_j} - \frac{\partial^2}{\partial x_j x_j}A_i = [\vec{\nabla}(\vec{\nabla}\cdot\vec{A}) - \vec{\nabla}^2\vec{A}]_i
\end{aligned}$$

where I have freely exchanged the order of differentiation when it suited me.

Equation (4.33) let's us show that Maxwell's Equations predict the existence of electromagnetic waves. Let's see how this works. If we just talk about some region in space where there are no charges or currents, call it the "vacuum", then Maxwell's Equations become

$$\vec{\nabla}\cdot\vec{E}=0 \qquad \vec{\nabla}\cdot\vec{B}=0 \qquad \vec{\nabla}\times\vec{E}=-\frac{1}{c}\frac{\partial\vec{B}}{\partial t} \qquad \vec{\nabla}\times\vec{B}=\frac{1}{c}\frac{\partial\vec{E}}{\partial t}$$

Take the curl of the third equation, invoke (4.33), and use the first equation to get

$$\vec{\nabla}\times(\vec{\nabla}\times\vec{E})=\vec{\nabla}(\vec{\nabla}\cdot\vec{E})-\vec{\nabla}^2\vec{E}=-\vec{\nabla}^2\vec{E}=-\frac{1}{c}\frac{\partial}{\partial t}\vec{\nabla}\times\vec{B}$$

Finally, use the fourth equation to replace $\vec{\nabla}\times\vec{B}$ with the time derivative of $\vec{E}$. After a little rearranging, you find

$$\frac{1}{c^2}\frac{\partial^2\vec{E}}{\partial t^2}-\vec{\nabla}^2\vec{E}=0 \tag{4.34}$$

This partial differential equation is called the *Wave Equation*. We will discuss solutions to the wave equation in Section 5.1, but it describes a field $\vec{E}(\vec{r},t)$ with a shape that moves in time, unchanged, at speed c.

Equation (4.34) looks a little weird because it is a partial differential equation that is to be solved for a *vector* function $\vec{E}(\vec{r},t)$. Let's try writing $\vec{E}(\vec{r},t)=\hat{\imath}f(z,t)$, which describes an electric field that is "linearly polarized in the x-direction." Inserting this (4.34) gives us

$$\frac{1}{c^2}\frac{\partial^2 f}{\partial t^2}-\frac{\partial^2 f}{\partial z^2}=0$$

which is a bit more tractable. We will see in Section 5.1 that this equation describes a wave moving in the z-direction.

You will do much more with electromagnetic waves in your E&M courses. It all boils down, though, to using Maxwell's Equations to derive the relevant PDE's and then solving them, given initial and boundary conditions.

4.4 Two important vector fields

Let's pause briefly to talk about two particular vector field forms that I'll call $\vec{B}(\vec{r})$ and $\vec{E}(\vec{r})$. Describing $\vec{B}(\vec{r})$ in Cartesian and *cylindrical* polar coordinates,

$$\vec{B}(\vec{r})=a\frac{-\hat{\imath}y+\hat{\imath}x}{x^2+y^2}=a\frac{\hat{\phi}}{r} \tag{4.35}$$

I will define the field $\vec{E}(\vec{r})$ in Cartesian and *spherical* polar coordinates as

$$\vec{E}(\vec{r})=a\frac{\hat{\imath}x+\hat{\jmath}y+\hat{k}z}{(x^2+y^2+z^2)^{3/2}}=a\frac{\hat{r}}{r^2} \tag{4.36}$$

In both of these equations, a just represents some constant.

I will leave it as a homework problem to calculate $\vec{\nabla} \times \vec{B}$ and $\vec{\nabla} \cdot \vec{E}$. Not to spoil the suspense, but you will find that the answer is zero in both cases. This is despite the fact that, if you make VectorPlot plots of these, $\vec{B}(\vec{r})$ will clearly look like it "curls" and $\vec{E}(\vec{r})$ will very obviously "diverge."

In fact, if you try testing the surface theorems on these fields, you will get nonzero results! The easiest way to do this is using a circle centered at the origin in the xy plane as the closed loop for $\vec{B}(\vec{r})$, and a sphere centered on the origin for the closed surface for $\vec{E}(\vec{r})$. For each of these, the surface integrals are trivial if you use the appropriate polar coordinate system.

This looks like violations of Stokes' Theorem and Gauss' Theorem, but in fact they are not. There is a subtlety that should be obvious when you think about it. It will take us a little while to get to the mathematics we need to write down what I'm talking about, but I wanted to get you thinking about it first.

4.5 Partial Differential Equations

Partial Differential Equations, or PDE's, are differential equations with more than one independent variable, so involve partial derivatives with respect to those variables. You will see them everywhere in Physics, from electromagnetism, to quantum mechanics, and continuum mechanics. We can only barely have a discussion about PDE's in general, but we will highlight the most common techniques used to solve them.

Probably the most important difference, effectively, between PDE's and ODE's is that the boundary conditions are much more involved and can lead to much more general solutions. We will be dealing with linear PDE's only, so superposition will still be valid. *This will be key to determining linear combinations of solutions that satisfy boundary conditions.*

It's good to illustrate these points with a problem that looks simple, but shows that boundary conditions are critical to finding even the general form of a solution. Consider the PDE

$$\frac{\partial f}{\partial x} = x \frac{\partial f}{\partial y}$$

to be solved for the function $f(x, y)$. You can easily verify (with MATHEMATICA if you want to) that the following are *all* solutions to this PDE:

$$\begin{aligned} f_1(x, y) &= x^4 + 4(x^2 y + y^2 + 1) \\ f_2(x, y) &= \sin x^2 \cos 2y + \cos x^2 \sin 2y \\ f_3(x, y) &= \frac{x^2 + 2y + 2}{3x^2 + 6y + 5} \end{aligned}$$

That seems odd until you realize that all three are functions of $z = x^2 + 2y$. That is,

$$\begin{aligned} f_1(x,y) &= z^2 + 4 \\ f_2(x,y) &= \sin z \\ f_3(x,y) &= \frac{z+2}{3z+5} \end{aligned}$$

Indeed, for any function $g(z)$,

$$\frac{\partial g}{\partial x} = g'(x)\frac{\partial z}{\partial x} = 2xg'(x) \qquad \text{and} \qquad x\frac{\partial g}{\partial y} = xg'(x)\frac{\partial z}{\partial y} = 2xg'(x)$$

so any function $f(x,y) = g(z)$ solves the PDE. Which of these infinite possible forms of the solution you pick, though, will depend on what boundary conditions you need to satisfy.

4.5.1 Separation of variables

Most if not all of the PDE's you'll need to solve in your studies of Physics will be linear and second order, and most if not all of these can be solved using a technique called *Separation of Variables*. This section goes through the principles of this technique, and it will be applied in various places throughout the rest of this course. You will see it used often in your courses on electromagnetism and quantum mechanics.

Separation of variables turns a partial differential equation for a function in terms of two or three independent variables (like x, y, and z, or r, θ, and ϕ into a set of separate ordinary differential equations, one for each of the independent variables. Suppose we are looking to solve a PDE for a function $f(\vec{r}) = f(x,y,x)$. The first step is to write

$$f(x,y,z) = X(x)Y(y)Z(z)$$

and insert into the PDE. It is generally possible to arrange the terms in a way that some constant or constants can be used to isolate the different ODE's.

We will illustrate this idea in a moment, but first an important point: What coordinate system you use is probably most dependent on what are the boundary conditions. If you have $f(\mathbf{r})$ and its partial derivatives defined along the boundaries of a rectangle or rectangular box, then you likely want to use Cartesian coordinates. If they are defined along the boundaries of a sphere, then you are apt to use spherical coordinates.

Each problem is different, though, and you have to consider it carefully before you plow forward. Remember that you still have existence and uniqueness to help you out. Any way that you can find a solution to the PDE that satisfies the boundary conditions, will give you, essentially, the right solution.

So, instead of writing down any general rules, let's solve a specific problem so that you can see how this technique works. Let's solve the partial differential equation

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial^2 f}{\partial y^2}$$

for the function $f(x, y)$ subject to the boundary conditions

$$f(0, y) = f(a, y) = f(x, 0) = f(x, a) = 0$$

where a is a positive constant. That is, the region of validity of the solution is the square of side length a in the first quadrant.

If you think about it, there is a more or less obvious solution to the differential equation. If $f(x, y) = g(z)$ with $z = x \pm y$ for any function $g(z)$, then the PDE is satisfied. In fact, a general solution would be

$$f(x, y) = g_1(x - y) + g_2(x + y)$$

where g_1 and g_2 are arbitrary functions. However, it's not so obvious how to choose these functions so that the boundary conditions are satisfied.

For this, we turn to a solution that makes use of Separation of Variables. As suggested above, we write $f(x, y) = X(x)Y(y)$ which gives

$$\frac{d^2X}{dx^2}Y = X\frac{d^2Y}{dy^2} \qquad \text{so} \qquad \frac{1}{X}\frac{d^2X}{dx^2} = \frac{1}{Y}\frac{d^2Y}{dy^2}$$

which is a peculiar type of equation. The left side depends only on x, while the right side depends only on y. Nevertheless, the two sides have to be equal to each other! The only way this happens if both sides are equal to a constant.

Let's call this constant $-k^2 < 0$. (You'll see shortly that this choice for the constant allows us to satisfy the boundary conditions.) The PDE has now split into two ODE's, as advertised. The two ODE's are

$$X''(x) = -k^2X(x) \qquad \text{and} \qquad Y''(y) = -k^2Y(y)$$

whose solutions are now very well known to you, namely

$$X(x) = A_x \cos kx + B_x \sin kx \qquad \text{and} \qquad Y(y) = A_y \cos ky + B_y \sin ky$$

where A_x, B_x, A_y, and B_y are constants. The boundary conditions imply that

$$X(0) = 0 = Y(0) \qquad \text{and} \qquad X(a) = 0 = Y(a)$$

The first pair of equations say that $A_x = 0 = A_y$, so the solution to the PDE has the form

$$f(x, y) = C \sin kx \sin ky$$

where $C = B_xB_y$. In order for $f(a, y) = 0 = f(x, a)$, and to avoid the trivial solution with $C = 0$, we need to set $k = n\pi/a$ were $n \in \mathbb{Z}^+$ is a positive integer. (A negative integer would give a redundant function, and $n = 0$ leads to the trivial solution.) Therefore

$$f(x, y) = C \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{n\pi y}{a}\right)$$

where the constant C would have to be determined by some additional constraint. If you recall the trigonometric identity

$$\sin\alpha \sin\beta = \frac{1}{2}\left[\cos(\alpha-\beta) - \cos(\alpha+\beta)\right]$$

then you see that, indeed, $f(x,y)$ is a linear combination of functions of $x \pm y$.

This worked out nicely because I picked boundary conditions that were amenable to a solution with separation of variables. Luckily, most of the physics problems you will face work out nicely like this. For other cases, not uncommon in various types of modeling of systems, you may need to resort to numerical solutions.

4.5.2 Heat conduction in one dimension

A common problem in the physical and life sciences, including engineering, is the diffusion of heat (or equivalent entity) through a medium over time. This process is governed by a partial differential equation of the form

$$\vec{\nabla}^2 f = k\frac{\partial f}{\partial t} \tag{4.37}$$

where $f(\vec{r},t)$ is the temperature field and k is a positive constant, called the *diffusivity*. This equation implies that there is no heat source in the medium, but that its internal energy can only get redistributed by the transfer of heat. We refer to (4.37) as the *heat equation* or *diffusion equation*.

In one spatial dimension x, (4.37) becomes

$$\frac{\partial^2 f}{\partial x^2} = k\frac{\partial f}{\partial t} \tag{4.38}$$

which would govern, for example, the temperature distribution $f(x,t)$ for position along a rod as a function of time. If the rod has length ℓ, its ends are held at fixed temperatures, and its initial temperature distribution is some function $u(x)$ for $0 \le x \le \ell$, then you have a prototypical PDE boundary and initial value problem to solve.

We should think for a minute about the physical system (4.38) would describe. After some time, we expect that the rod would come to thermal equilibrium with its "surroundings", namely the source or sink of heat to which each endpoint is attached. In equilibrium, the temperature $f(x,t)$ would no longer change with time, and the right side of (4.38) would be zero. The resulting (ordinary) differential equation is trivial to solve. You get

$$f(x, t\to\infty) = ax + b$$

where the constants a and b are set by the temperatures at the ends of the rod. Something in the time dependence of $f(x,t)$ must have the time dependence disappear after a long time.

A natural approach to solving (4.38) for the temperature of a rod, is to use Separation of Variables and write $f(x,t) = X(x)T(t)$. In this case (4.38) becomes

$$\frac{1}{X}\frac{d^2X}{dx^2} = k\frac{1}{T}\frac{dT}{dt}$$

and we need to set both sides equal to a constant. If we make this constant negative, for example $-\alpha^2$, then $T(t)$ will be a decaying exponential, which sounds like it fits the bill for a disappearing time dependence.

We would also find that $X(x)$ is a linear combination of sines and cosines. Enforcing fixed temperatures at the end of the rod will have us write the argument of the sines and cosines as some integer times π/ℓ. In order to satisfy the initial condition that $f(x,0 = u(x)$ for an arbitrary $u(x)$, we would have to find the linear combinations of all of the n-valued sines and cosines that give you $u(x)$.

This process of adding up sines and cosines to give you some arbitrary function was invented in the early 19th century by Joseph Fourier, and is the subject of Chapter 5. According to lore, Fourier developed this technique to solve the problem of how to best dissipate heat in the cannons of Napoleon Bonaparte's army. We'll use a more traditional approach to develop Fourier Series, and then the Fourier Transform, namely standing waves on a string.

Chapter 5

Fourier Analysis

Fourier Analysis is based on the fact – which we won't prove – that pretty much any function can be represented by an infinite sum, or perhaps an integral, of sines and cosines. Although applicable to any number of physical problems (for example, heat conduction, as mentioned in Section 4.5.2), we will illustrate it using solutions to the Wave Equation.

Much of this chapter should be review from Wave Physics.

5.1 Waves on a Stretched String

We are going to start this discussion by considering the motion of a string, stretched tightly. We'll say the string is in the horizontal direction and moves only in the vertical direction, because it never bends by very much, but gravity is irrelevant. We are only going to care about the vertical motion due to the tension in the string. What we'll find is that the motion of the string is governed by the same partial differential equation that governs electromagnetic waves, for example (4.34).

5.1.1 Derivation of the equation of motion

Imagine a string stretched across space. We will derive an equation that governs the up-and-down motion of the string, assuming that it never bends by very much. We will do this by considering tiny piece of the string and applying Newton's Second Law. The only forces on this piece of string that will concern us are the tensions on the piece from each of its two ends.

Figure 5.1 shows a small piece of stretched string. We measure the position along the horizontal direction as x, and the shape of the string at any time t is $u(x,t)$. We assume that θ is always very small so that the string only moves vertically.

In order to apply Newton's Second Law, let's first analyze the vertical forces on the string.

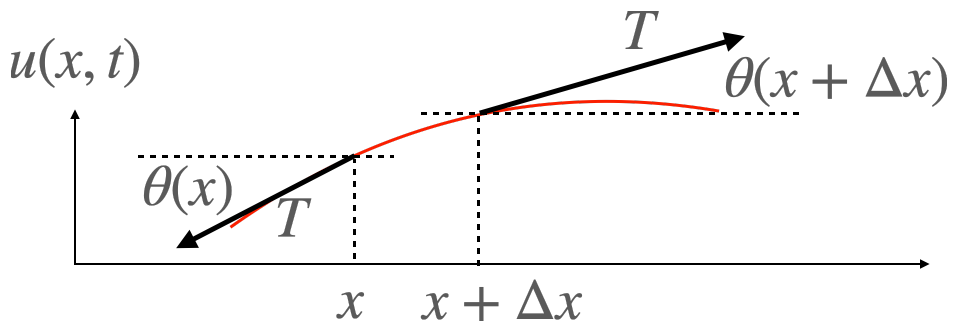


Figure 5.1: A small piece of a string (drawn in red) acted on by the tension forces from each end. We use θ to measure the angle of the string with respect to the horizontal at each end.

These are

$$-T\sin\theta \approx -T\theta \approx -T\tan\theta = -T\left.\frac{\partial u}{\partial x}\right|_x$$

on the left, and

$$T\sin\theta \approx T\theta \approx T\tan\theta = T\left.\frac{\partial u}{\partial x}\right|_{x+\Delta x}$$

on the right. Therefore, the sum of forces acting on this small piece of string is

$$\sum F_y = -T\left.\frac{\partial u}{\partial x}\right|_x + T\left.\frac{\partial u}{\partial x}\right|_{x+\Delta x} = T\left[\left.\frac{\partial u}{\partial x}\right|_{x+\Delta x} - \left.\frac{\partial u}{\partial x}\right|_x\right]$$

Now if we let μ be the linear mass density of the string, then the mass of this small piece is $\mu\Delta x$, and Newton's Second Law for the vertical motion of the piece of string is

$$\mu\Delta x\frac{\partial^2 u}{\partial t^2} = T\left[\left.\frac{\partial u}{\partial x}\right|_{x+\Delta x} - \left.\frac{\partial u}{\partial x}\right|_x\right] \qquad \text{or} \qquad \frac{\mu}{T}\frac{\partial^2 u}{\partial t^2} = \frac{1}{\Delta x}\left[\left.\frac{\partial u}{\partial x}\right|_{x+\Delta x} - \left.\frac{\partial u}{\partial x}\right|_x\right]$$

It is easy to see that the constant μ/T on the left has dimensions of velocity^2. That is

$$\frac{[\mu]}{[T]} = \frac{ML^{-1}}{MLT^{-2}} = \frac{1}{(L/T)^2}$$

So, let's write $v^2 = T/\mu$. Also, as the piece of string gets smaller and smaller, that is $\Delta x \to 0$, the right side just becomes the second partial derivative with respect to x. In other words, the motion of the string is governed by the partial differential equation

$$\frac{1}{v^2}\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \qquad \text{or} \qquad \frac{\partial^2 u}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2 u}{\partial t^2} = 0 \tag{5.1}$$

This is known as the *Wave Equation* and it shows up in many different areas of physics. We have already seen that it is implied by Maxwell's Equations in Section 4.3.4.

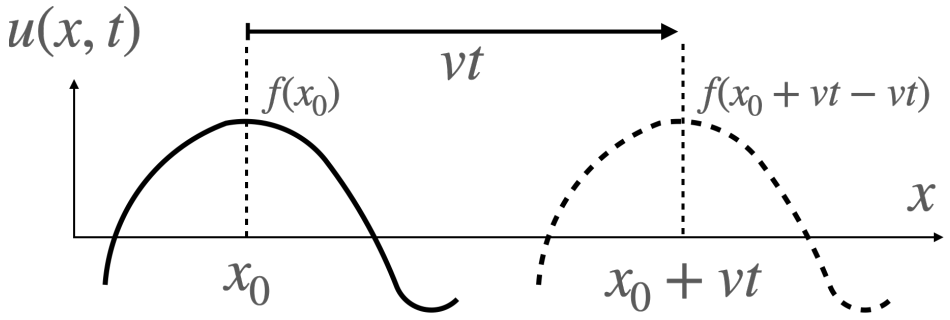


Figure 5.2: Motion of a string according to (5.1) for the part of the general solution (5.2) that is $f(x - vt)$. At $t = 0$, the height of the string at a point x_0 is $f(x_0)$, and at a finite time t, the height of the wave at $x_0 + vt$ is the same value $f(x_0)$.

5.1.2 General solution of the wave equation

There are many different forms for the function $u(x, t)$ that solves (5.1) that depend on the initial and boundary conditions. However, we can immediately see a specific general form of the solution that gives us good intuition as to what's going on.

First, realize that (5.1) is a linear PDE. That means that if $u_1(x, t)$ and $u_2(x, t)$ are both solutions, then any linear combination $c_1u_1(x, t) + c_2u_2(x, t)$ is also a solution.

Now it is not hard to see that any function of $z = x - vt$ is a solution to (5.1). That is, $u(x, t) = f(z) = f(x - vt)$ will be a solution for any (differentiable) function $f(z)$. The same is true for any function $g(x + vt)$. In other words, the general solution to (5.1) is any function of the form

$$u(x, t) = f(x - vt) + g(x + vt) \tag{5.2}$$

This general form has a lovely physical interpretation. Consider first the motion in time of the function $f(x - ct)$, shown in Figure 5.2. Whatever the shape is at $t = 0$, that is $f(x)$, it is reproduced exactly at a finite time t except that it is translated to the right by an amount vt. In other words, it moves to the right with a speed v.

in other words, the first term in the solution (5.2) represents a "wave moving to the right with speed v." The second term, that is $g(x + vt)$ represents, similarly, a "wave moving to the left with speed v.

It is not hard to show that if you start at time $t = 0$ with some arbitrary string shape $f(x)$, with the string at rest, then the solution is that the shape splits into two pieces, one moving to the right and the other moving to the left. This will be a homework problem.

Another easy solution to the wave equation is for a string that is fixed at one end, or allowed to move freely at one end. These cases correspond to the boundary conditions that $u(0, t) = 0$ or $\partial u(x, t)/\partial x|_{x=0} = 0$, assuming the end to be at $x = 0$. In each case, you find that the wave is "reflected" from the end, but the characteristics of the reflection are different for the two cases. This will also be a homework problem.

5.2 Standing waves

Now we are going to investigate solutions to (5.1) with some specific boundary conditions, namely that the ends of the string are fixed and cannot vibrate. The result is a phenomenon that we refer to as *standing waves*.

You likely solved this in your Wave Physics course, but with the boundaries of the string at $x = 0$ and $x = L$. This simplifies things because the solutions are all sine functions. I will go through the solution here again, but with the boundaries at $x = \pm L/2$. This will allow us to exploit the symmetry about $x = 0$, let us show off the use of complex notation, and facilitate taking the limit $L \to \infty$ when we get to the Fourier Transform.

Our goal is to find a $u(x,t)$ that solves (5.1) subject to the boundary conditions

$$u\left(-\frac{L}{2},t\right) = 0 = u\left(\frac{L}{2},t\right) \tag{5.3}$$

We will worry about initial conditions later. A good approach is separation of variables, so, recalling Section 4.5.1, we write $u(x,t) = X(x)T(t)$ leading to the equations

$$\frac{1}{v^2}\frac{1}{T}\frac{d^2T}{dt^2} = \frac{1}{X}\frac{d^2X}{dx^2} = -k^2 \tag{5.4}$$

where the constant $-k^2 < 0$ is chosen, as we'll see in a moment, to meet the boundary conditions. It should be clear to you by now that the solution for $X(x)$ are sines and cosines, but it will be better for us to use Euler's Formula to write

$$X(x) = Ae^{ikx} + Be^{-ikx}$$

The boundary conditions are obviously satisfied by setting $X(-L/2) = 0 = X(L/2)$, that is

$$\begin{aligned} Ae^{-ikL/2} + Be^{ikL/2} &= 0 \\ Ae^{ikL/2} + Be^{-ikL/2} &= 0 \end{aligned}$$

to be solved for A and B. We've seen this kind of problem before, for example in solving for the modes of the coupled oscillator in Section 3.7.1. The solution would be $A = B = 0$ unless we make these two equations into one equation by making the ratio of coefficients equal to unity. That is

$$\frac{e^{-ikL/2}}{e^{ikL/2}} = \frac{e^{ikL/2}}{e^{-ikL/2}} \qquad \text{or} \qquad e^{-ikL} = e^{ikL} \qquad \text{or} \qquad e^{2ikL} = 1$$

which means that $kL = n\pi$ where n is a positive integer. (Since $\pm k$ both give solutions, we might as well just let n be positive.) Therefore we have determined that

$$X(x) = A_n e^{in\pi x/L} + B_n e^{-in\pi x/L}$$

where $n \in \mathbb{Z}^+$, and A_n and B_n are (complex) constants that need to be determined from the initial conditions.

Separation of variables also gives us the differential equation to solve for $T(t)$, namely

$$\frac{d^2T}{dt^2} = -k^2v^2T(t) = -\left(\frac{n\pi v}{L}\right)^2 T(t)$$

This determines the form of $T(t)$ to be

$$T(t) = \sin\left(\frac{n\pi vt}{L}\right) \qquad \text{or} \qquad T(t) = \cos\left(\frac{n\pi vt}{L}\right)$$

or some linear combination of the two. At this point will make a simplifying assumption. For the sake of avoiding unnecessary complication, *we will assume that any problem we want to solve has the string at rest at* $t = 0$. This assumption implies that $T'(0) = 0$, so we choose the cosine option for $T(t)$.

Therefore, we determined the shape of the string to be

$$u(x,t) = \left[A_n e^{in\pi x/L} + B_n e^{-in\pi x/L}\right] \cos\left(\frac{n\pi vt}{L}\right) \tag{5.5a}$$

$$\text{or} \qquad u(x,t) = \left[\tilde{A}_n \cos\left(\frac{n\pi x}{L}\right) + \tilde{B}_n \sin\left(\frac{n\pi x}{L}\right)\right] \cos\left(\frac{n\pi vt}{L}\right) \tag{5.5b}$$

where $\tilde{A}_n = A_n + B_n$ and $\tilde{B}_n = i(A_n - B_n)$. Which form we use depends on which problem we want to solve. Clearly (5.5b) is best if we are trying to determine the shape of a physical string. However, we'll see that (5.5a) is more useful in general, and will in fact lead us in new directions.

Recall that we decided we needed $n \geq 1$. We cannot have $n = 0$ because that would imply that $u(x, t = 0)$ is a constant that must be zero because of our boundary conditions. We also realized that $n < 0$ is redundant, so we discarded. We will revisit these conditions later.

Now we are armed with the general solution (5.5) so we should be able to solve the mathematical problem posed by (5.1) with boundary conditions (5.3). All we need to do is match this general form to the initial condition $u(x, 0) = f(x)$. (Remember that we settled on (5.5) by requiring that $\dot{u}(x, 0) = 0$.)

But how do we do that, for an arbitrary $f(x)$? If $f(x)$ is a sine or cosine function or some linear combination of both, equal to zero at $x = \pm L/2$, then it is easy. We would just pick the appropriate value of $\tilde{A}_n$ and $\tilde{B}_n$. In general, of course, we'd need to write the solution as a sum over all possible values of n, and somehow figure out a formula for $\tilde{A}_n$ and $\tilde{B}_n$ (or A_n and B_n) in terms of n. The result is called a *Fourier Series* and that's what we take on next.

5.3 Fourier Series

As the story goes, Joseph Fourier developed the idea of expanding a function in terms of sines and cosines in order to solve the heat conduction equation in Section 4.5.2. As we just saw in Section 5.2, it is also a path for solving the problem of standing waves on a string. These are important hints that this is a generally useful technique.

So let's go through the analysis using more general mathematics. After that, we'll take a moment to apply what we have to the problem of standing waves on a string.

It apparently took some time for Fourier's ideas to be accepted. The notion that an arbitrary function can be expanded in terms of sines and cosines is not clearly true, and there is some interesting mathematics that goes along with it. I think mathematicians refer to the need to prove "completeness", but we're not going to get into the details. Our point of view will be that if we can find a way to calculate the expansion coefficients, then our job is done.

5.3.1 Expansion in terms of harmonics

Referring to standing waves on a string for a moment, our problem comes down to writing the initial condition $u(x,0) = f(x)$ in terms of a sum over n of the expressions in (5.5). We'll work with the form in (5.5a) and write

$$f(x) = \sum_{n=1}^{\infty} \left[A_n e^{ik_n x} + B_n e^{-ik_n x} \right]$$

which we'll call an *expansion in terms of harmonics*. It is important to note that

$$-\frac{L}{2} \le x \le \frac{L}{2} \tag{5.6}$$

In fact, by enforcing that $f(x) = 0$ at $x = \pm L/2$, we found that $k_n L = n\pi$.

Before plowing ahead, let's make some observations of, and changes in, the harmonic expansion above. Firstly, we have excluded $n = 0$ because that term contributes a constant to $f(x)$, and the standing wave boundary conditions implied that constant had to be zero. If we want to consider more general forms of $f(x)$, then we can relax that requirement and include $n = 0$ in the sum.

Note also that the terms for A_n and B_n just flip signs in the exponent, so if we let n be negative, then we only have to do one of the sums. So, now the sum harmonic expansion is written as

$$f(x) = \sum_{n=-\infty}^{\infty} A_n e^{ik_n x}$$

We will also generalize the boundary conditions. Instead of enforcing $f(x) = 0$ at $x = \pm L/2$, let's use "periodic boundary conditions." That is, the initial shape $f(x)$ isn't constrained

to be between $\pm L/2$, but the shape does repeat periodically with period a. (As we'll see later, we can adapt this to a string with ends fixed at $u(\pm L/2, t) = 0$ with $a = 2L$.) Mathematically, this means

$$f(x + a) = f(x)$$

and this gives us a slightly different expression for k_n, namely

$$e^{ik(x+a)} = e^{ikx} \qquad \text{so} \qquad e^{ika} = 1 \qquad \text{or} \qquad ka = 2\pi n$$

for some integer n. Therefore $k = k_n = n2\pi/a$ and we write our general mathematics problem as

$$f(x) = \sum_{n=-\infty}^{\infty} A_n e^{2in\pi x/a} \tag{5.7}$$

where the goal is to find an expression for A_n given an arbitrary $f(x)$.

We get a strong hint on how to find the A_n by integrating both sides over x. Integrating over one period using the region $-a/2 \le x \le a/2$,

$$\begin{aligned} \int_{-a/2}^{a/2} f(x)\,dx &= \sum_{n=-\infty}^{\infty} A_n \int_{-a/2}^{a/2} e^{2in\pi x/a}\,dx \\ &= \sum_{n=-\infty}^{\infty} A_n \frac{a}{2in\pi}\left[e^{in\pi} - e^{-in\pi}\right] = \sum_{n=-\infty}^{\infty} A_n \frac{a}{n\pi}\sin(n\pi) \end{aligned}$$

Now $\sin(n\pi) = 0$ for any integer n, so it looks like every term on the right side is zero. However, we have to be careful about the $n = 0$ term. In this case

$$\int_{-a/2}^{a/2} f(x)\,dx = A_0 \int_{-a/2}^{a/2} (1)\,dx = A_0 a \qquad \text{or} \qquad A_0 = \frac{1}{a}\int_{-a/2}^{a/2} f(x)\,dx$$

and we see that A_0 is just the average value of the function over one period. This makes good sense. If $n \neq 0$, then the exponential terms are just sines and cosines, all of which integrate to zero over one period.

This tells us how to find the other A_n. Multiply $f(x)$ by $e^{-2im\pi x/a}$ before integrating, where m is some integer. This gives us

$$\int_{-a/2}^{a/2} e^{-2im\pi x/a} f(x)\,dx = \sum_{n=-\infty}^{\infty} A_n \int_{-a/2}^{a/2} e^{i(n-m)2\pi x/a}\,dx = \sum_{n=-\infty}^{\infty} A_n \frac{a}{(n-m)\pi}\sin[(n-m)\pi]$$

and we have the same situation we had for $m = 0$. That is, every term in the expansion is zero except when $n = m$, in which case

$$\int_{-aL/2}^{a/2} e^{-2im\pi x/a} f(x)\,dx = A_m a$$

Of course, m is just a dummy index, so we have the general expression

$$A_n = \frac{1}{a}\int_{-a/2}^{a/2} e^{-2in\pi x/a} f(x)\,dx \tag{5.8}$$

which is good for all integers n. As far as we're concerned, this confirms that the harmonic expansion (5.7) is valid.

Let's try a simple example, namely $f(x) = \sin(2\pi x/a)$, to check the formalism. Note that this $f(x)$ has the correct period, namely $f(x+a) = f(x)$. Write

$$\sin\left(\frac{2\pi x}{a}\right) = \frac{1}{2i}e^{2i\pi x/a} - \frac{1}{2i}e^{-2i\pi x/a}$$

and use (5.8) to get the coefficients

$$A_n = \frac{1}{2ia}\left[\int_{-a/2}^{a/2} e^{2i\pi(1-n)x/a}\,dx - \int_{-a/2}^{a/2} e^{2i\pi(-1-n)x/a}\,dx\right]$$

where both integrals are zero unless $n = \pm 1$. In those cases, we have

$$A_1 = \frac{1}{2ia}\int_{-a/2}^{a/2}(1)\,dx = \frac{1}{2i} \qquad \text{and} \qquad A_{-1} = -\frac{1}{2ia}\int_{-a/2}^{a/2}(1) = -\frac{1}{2i}$$

There are only two terms, therefore, in the expansion (5.7) and we have

$$f(x) = \frac{1}{2i}e^{2i\pi x/a} - \frac{1}{2i}e^{-2i\pi x/a} = \sin\left(\frac{2\pi x}{a}\right)$$

which is of course correct.

A more interesting example is the "sawtooth" function $f(x) = x/a$ for $-a/2 \le x \le a/2$ and which repeats with period a. Maybe for homework. Also the "square wave", namely

$$\begin{aligned} f(x) &= 1 \qquad \text{for} \qquad -\frac{a}{4} \le x \le \frac{a}{4} \\ \text{and} \qquad &= -1 \qquad \text{for} \qquad -\frac{a}{2} \le x \le -\frac{a}{4} \qquad \text{and} \qquad \frac{a}{4} \le x \le \frac{a}{2} \end{aligned}$$

and repeating with period a. Maybe these are too difficult, not sure.

5.3.2 Standing wave solution

We can now use the harmonic expansion (5.7), with coefficients given by (5.8), to solve the problem of standing waves on a string, from Section 5.2. To review, for a stretched string with ends fixed at $x = \pm L/2$, we found the class of solutions (5.5) for different $n \ge 1$. The

issue now is how to match these to a solution for a string with initial shape $u(x,0) = f(x)$. We will do this by starting with (5.7) to find the coefficients $\tilde{A}_n$ and $\tilde{B}_n$ in (5.5b).

The first issue we face is to find the relationship between the "periodicity" a and the length L of the string. Recall that "fixed ends" means $f(\pm L/2) = 0$. It is tempting to just write $a = L$, but we have to be careful. Certainly, we can have the shape $f(x)$ just repeat itself, going to zero at every point beyond the ends of the string with period L. However, this is not general enough. It is also possible for the shape $f(x) \to -f(x)$ past the ends of the strings. For example, the function $\sin(2\pi x/L) = 0$ at $x = \pm L/2$ and has period L, but the function $\cos(\pi x/L)$ also goes to zero at $x = \pm L/2$ but has period $2L$.

Therefore, to start with (5.7) means we pick $a = 2L$. That is, we write

$$f(x) = \sum_{n=-\infty}^{\infty} A_n e^{in\pi x/L} \qquad \text{where} \qquad A_n = \frac{1}{2L}\int_{-L}^{L} e^{-in\pi x/L} f(x)\,dx \tag{5.9}$$

Of course, $f(x)$ is a real function since we are talking the motion of a physical string, so it's better to write the expansion in terms of sines and cosines. We also split the sum according to the sign of n and write

$$\begin{aligned}
f(x) &= A_0 + \sum_{n=1}^{\infty} \left[A_n e^{in\pi x/L} + A_{-n} e^{-in\pi x/L}\right] \\
&= A_0 + \sum_{n=1}^{\infty} \left[\tilde{A}_n \cos\left(\frac{n\pi x}{L}\right) + \tilde{B}_n \sin\left(\frac{n\pi x}{L}\right)\right] \\
\text{where} \qquad \tilde{A}_n = A_n + A_{-n} &= \frac{1}{L}\int_{-L}^{L} \cos\left(\frac{n\pi x}{L}\right) f(x)\,dx \\
\text{including} \qquad A_0 = \frac{1}{2}\tilde{A}_0 &= \frac{1}{2L}\int_{-L}^{L} f(x)\,dx \\
\text{and} \qquad \tilde{B}_n = i(A_n - A_{-n}) &= \frac{1}{L}\int_{-L}^{L} \sin\left(\frac{n\pi x}{L}\right) f(x)\,dx
\end{aligned}$$

which is the form (5.5b) but now we have expressions for the coefficients.

These relations are correct (so far as I know) but they are a little inconvenient for describing a physical string. The variable x doesn't measure position along the string, because it extends over a length $2L$, and $f(x)$ is a function which connects on the physical string, but extends beyond its endpoints. So, let's define the variable

$$y = \frac{x + L}{2}$$

which extends from 0 to L so measures position along the physical string. Since

$$\cos\left(\frac{n\pi x}{L}\right) = (-1)^n \cos\left(\frac{2n\pi y}{L}\right) \qquad \text{and} \qquad \sin\left(\frac{n\pi x}{L}\right) = (-1)^n \sin\left(\frac{2n\pi y}{L}\right)$$

the expansion for the physical string becomes

$$\begin{aligned} g(y) &= \tilde{A}_0 + \sum_{n=1}^{\infty} \left[\tilde{A}_n \cos\left(\frac{2n\pi y}{L}\right) + \tilde{B}_n \sin\left(\frac{2n\pi y}{L}\right) \right] \\ \text{where} \qquad \tilde{A}_n &= (-1)^n \frac{2}{L} \int_0^L \cos\left(\frac{2n\pi y}{L}\right) g(y)\, dy \\ \text{and} \qquad \tilde{B}_n &= (-1)^n \frac{2}{L} \int_0^L \sin\left(\frac{2n\pi y}{L}\right) g(y)\, dy \end{aligned}$$

where $g(y) = f[(x + L)/2]$ describes the shape of the physical string.

This is getting messy. I'm not sure how to treat the need to be continuous nature of the boundary conditions at the ends, other than to deal differently with even and odd n. I'm bothered by the "physical string" business, and I don't know about these factors of $(-1)^n$. I think it is better to retreat, do the string the standard "easy" way in the Tuesday class, then the generalized Fourier expansion and then the Fourier transform in the Thursday class.

Standing waves the easy way

Let's do the conventional approach to solving for standing waves on a string, and stick to real functions. If we put the ends of the string at $x = 0$ and $x = L$, then the solution to (5.4) for $X()$ is best written as

$$X(x) = A\cos(kx) + B\sin(kx)$$

Enforcing $X(0) = 0$ gives $A = 0$. Enforcing $X(L) = 0$ gives $kL = n\pi$, so the standing wave solution (for a string that is initially at rest) looks like

$$u_n(x,t) = B_n \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi v t}{L}\right) \tag{5.10}$$

which is, essentially, (5.5b). Confronting the initial condition $u(x, 0) = f(x)$ leads to

$$f(x) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) \tag{5.11}$$

where the job is now to find the B_n. (Sometimes this is called the *Fourier Sine Series*.)
There is an easy to find the B_n by exploiting the orthogonality of the sine functions, that is

$$\begin{aligned} &\int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx = \int_0^L \frac{1}{2} \left\{ \cos\left[\frac{\pi(n-m)x}{L}\right] - \cos\left[\frac{\pi(n+m)x}{L}\right] \right\} dx \\ = \quad &\frac{L}{2\pi(n-m)} \sin\left[\frac{\pi(n-m)x}{L}\right]\Bigg|_0^L - \frac{L}{2\pi(n+m)} \sin\left[\frac{\pi(n+m)x}{L}\right]\Bigg|_0^L = 0 \end{aligned}$$

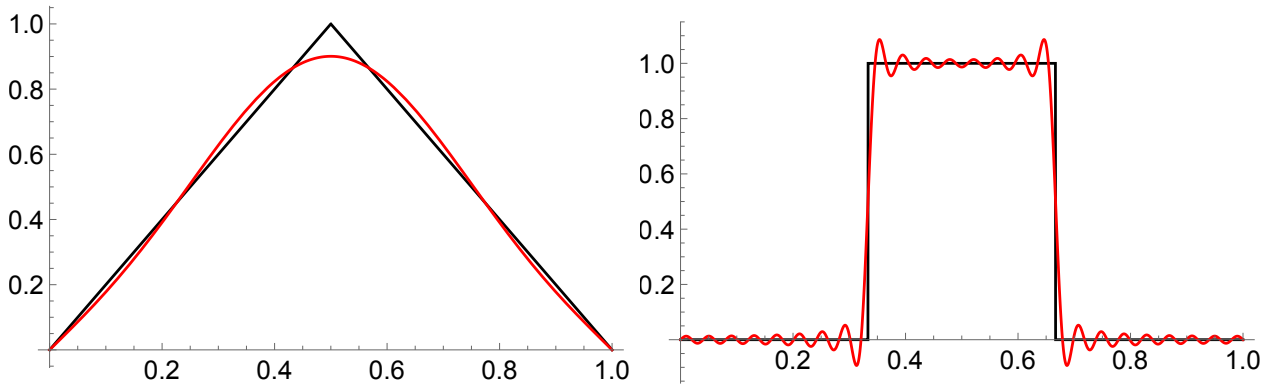


Figure 5.3: Fourier Sine decompositions of two waveforms. The triangle uses only the first four terms in the Fourier series, two of which are in fact zero. Even with so few terms, this approximation is reasonably good. The square wave, however, uses the first 50 terms, and there are still obvious discrepancies at the discontinuities.

for positive integers $n \neq m$. On the other hand, if $n = m$, then

$$\int_0^L \sin\left(\frac{m\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) = \frac{1}{2}\int_0^L \left[1 - \cos\left(\frac{2m\pi x}{L}\right)\right] = \frac{L}{2}$$

for any integer m. The simple way to write this result is

$$\int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx = \frac{L}{2}\delta_{nm}$$

Applying this to (5.11) gives

$$\int_0^L f(x) \sin\left(\frac{m\pi x}{L}\right) dx = \sum_{n=1}^{\infty} B_n \int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx = \sum_{n=1}^{\infty} B_n \frac{L}{2}\delta_{nm} = B_m \frac{L}{2}$$

In other words, switching back to the index n,

$$B_n = \frac{2}{L}\int_0^L f(x) \sin\left(\frac{n\pi x}{L}\right) dx \tag{5.12}$$

These are the coefficients of the Fourier Sine Series (5.11). Figure 5.3 shows two examples of Fourier Sine decompositions.

We can now return to our problem of finding the motion of standing waves on a string use (5.10) to write the solution for the motion of a string that is fixed at $x = 0$ and $x = L$ and which starts from rest with shape $u(x, 0) = f(x)$ as

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi v t}{L}\right) \tag{5.13}$$

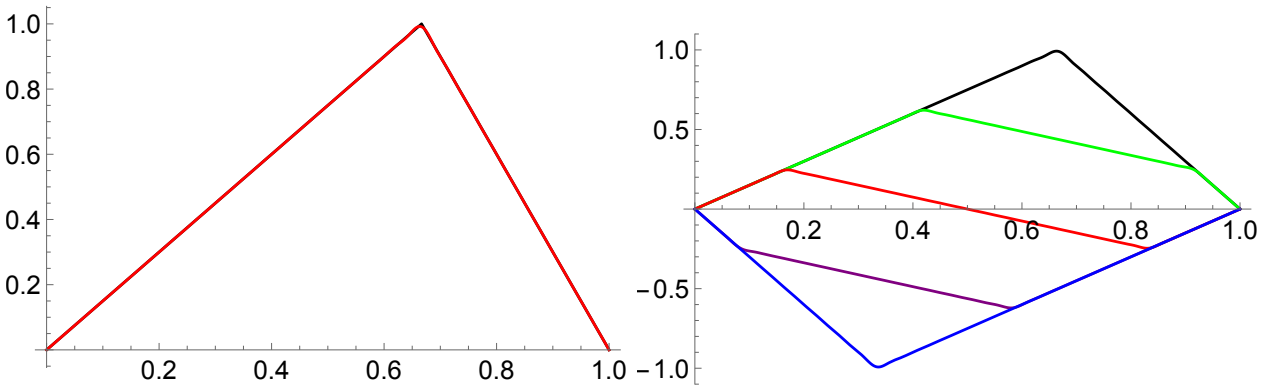


Figure 5.4: Fourier decomposition of a lopsided triangle, using the first 50 terms, along with its motion over time. The decomposition is almost indistinguishable from the exact triangle. The motion is traced out for $t = \delta(2\pi/\omega)$ where ω is the frequency of the lowest frequency component ($n = 1$) and $\delta = 0, 1/8, 1/4, 3/8, 1/2$.

where the coefficients B_n are given by (5.12). It is obvious that this has the shape $f(x)$ at $t = 0$ from our construction of the Fourier Sine Series, but notice also that the different n components oscillate with different frequencies $nv/2L$, so the shape will change as a function of time, as expected.

Figure 5.4 shows the motion of a lopsided triangle wave, using a large number of terms for the Fourier expansion. It is not obvious that this is the behavior you might expect, that is, the trapezoidal motion that maintains the skewness of the initial shape. This example actually makes a nice MATHEMATICA animation.

5.4 Parsevals theorem

I don't know that I will have time to cover this, but it is worthwhile at some point to mention the idea of "completeness." I also need to be careful of the ordering, because I think this is best done when we've done the generalized Fourier series, and the prior order may be changing if these notes are redone for another class.

I think the point is to prove that the average $|f(x)|^2$ over one period is just the sum of the Fourier coefficients squared. That is

$$\frac{1}{a}\int_{-a/2}^{a/2} |f(x)|^2 dx = \sum_{n=-\infty}^{\infty} |A_n|^2 \tag{5.14}$$

which is actually quite easy to prove. Just plow ahead and you get

$$\begin{aligned}\frac{1}{a}\int_{-a/2}^{a/2}|f(x)|^2dx &= \frac{1}{a}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}A_n^*A_m\int_{-a/2}^{a/2}e^{2i(m-n)\pi x/a}dx \\ &= \frac{1}{a}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}A_n^*A_m\,a\,\delta_{nm} = \sum_{n=-\infty}^{\infty}|A_n|^2\end{aligned}$$

The connection onto Quantum Mechanics is kind of nice, especially in terms of completeness, but it just seems like this is something that will have to wait for a later course.

5.5 Fourier Transform

In class I will first start with the general Fourier series, from Section 5.3.1. That is, start by considering a periodic function $f(x)$ with $f(x+a) = f(x)$, and an expansion

$$f(x) = \sum_{n=-\infty}^{\infty}A_n e^{ikx} \tag{5.15}$$

and end up with $k = 2n\pi/a$ and (5.8).

5.5.1 Taking the Limit of the General Fourier Series

We can now ask ourselves a nice little question. What happens if the periodicity a becomes infinite? You might suspect this can be useful for a "pulse" that is isolated in space and time. With $a \to \infty$, and n ranging over all the integers, k and n will become continuous variables. Realizing that $\Delta n = 1$, we can write

$$f(x) = \sum_{n=-\infty}^{\infty}A_n e^{ikx}\Delta n \underset{a\to\infty}{\longrightarrow} \int_{-\infty}^{\infty}A_n e^{ikx}\,dn = \int_{-\infty}^{\infty}[aA_n]e^{ikx}\,d\left(\frac{n}{a}\right) = \frac{1}{2\pi}\int_{-\infty}^{\infty}[aA_n]e^{ikx}\,dk$$

Now, from (5.8), we can write that

$$aA_n = \int_{-a/2}^{a/2}e^{-ikx}f(x)\,dx \underset{a\to\infty}{\longrightarrow} \int_{-\infty}^{\infty}e^{-ikx}f(x)\,dx$$

We redefine aA_n in the $a \to \infty$ limit to be the *Fourier Transform* of $f(x)$, that is

$$A(k) = \int_{-\infty}^{\infty}e^{-ikx}f(x)\,dx \tag{5.16}$$

The *Inverse Fourier Transform* goes the other way, giving $f(x)$ from $A(k)$, that is

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ikx}A(k)\,dk \tag{5.17}$$

There are different conventions on how to write the Fourier Transform and its inverse. Oftentimes, the signs of k are switched between the two (which pretty much amounts to switching x for k which you're of course free to do.) Sometimes the factor of $1/2\pi$ is "split", putting a factor of $1/\sqrt{2\pi}$ in front of both the transform and the inverse. Another variant is to include a factor of 2π in the exponent inside the integral.

We will use (5.16) and (5.17) as they are, but you should be aware that there is not a universal convention.

5.5.2 The Width of the Fourier Transform

The Fourier Transform will find most of its use when we consider "pulses," waveforms that are localized in space. For such a waveform $f(x)$, centered at $x = 0$, we can define a "width" using a definition inspired by the *standard deviation* from data analysis. (See Section 9.4.1.) If we call the width Δx, then

$$(\Delta x)^2 = \frac{1}{\mathcal{A}} \int_{-\infty}^{\infty} x^2 f(x)\, dx \qquad \text{where} \qquad \mathcal{A} = \int_{-\infty}^{\infty} f(x)\, dx \tag{5.18}$$

is the area under the pulse. Oftentimes, the pulse shape is defined so that $\mathcal{A} = 1$.

Of course, you can also determine the width of the Fourier transform of some localized $f(x)$. When we go through some examples of Fourier Transforms, you will see that if $f(x)$ is localized then so is its Fourier Transform. In fact, the "narrower" the pulse $f(x)$, the "wider" will be its Fourier Transform.

In fact, it is not always possible to calculate the width of the Fourier Transform. For many simple forms (two of which we'll see shortly), the integrals do not converge. We can nevertheless get a "geometric" interpretation of the widths from the shape of the transform.

5.5.3 Examples of Fourier Transforms

Let's first consider a simple square pulse. That is $f(x) = 1$ for $-a/2 \leq x \leq a/2$, and $f(x) = 0$ otherwise. It is simple to use (5.16) to calculate the Fourier Transform. We have

$$A(k) = \int_{-\infty}^{\infty} e^{-ikx} f(x)\, dx = \int_{-a/2}^{a/2} e^{-ikx}\, dx = \frac{1}{-ik}\left[e^{-ika/2} - e^{ika/2}\right] = \frac{2}{k}\sin\left(\frac{ka}{2}\right)$$

The function and transform are plotted in Figure 5.5. Similar to the way we saw the Fourier Sine Series behave, there are strong oscillations when the function has sharp discontinuities. Notice also that both pulses are localized, the square pulse more so than its transform.

Nevertheless, the product of the widths appears to be constant. Rather than do a precise calculation of the widths (which is in fact problematic for this particular Fourier Transform), just notice that the (geometric) width of the square pulse is $\Delta x = a$, whereas the width of

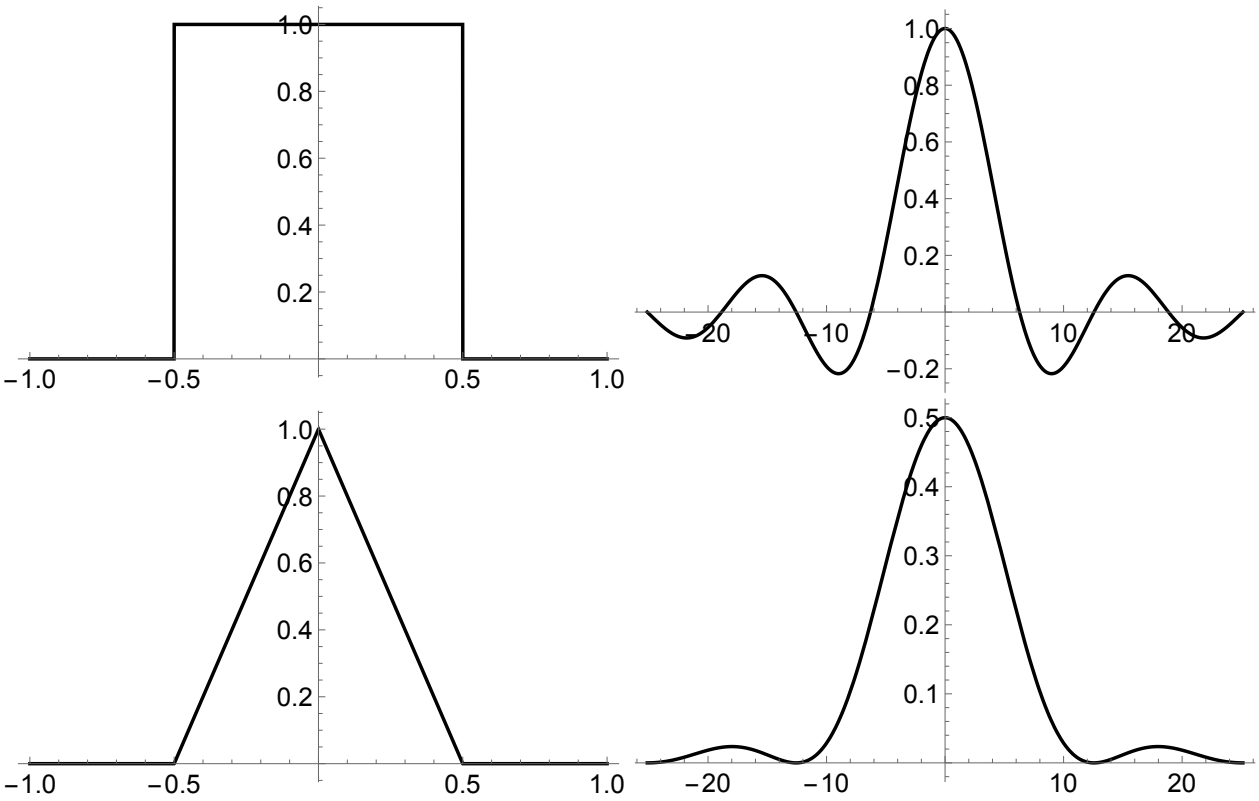


Figure 5.5: Examples of pulses and their Fourier Transforms. The top row shows a square pulse and the bottom shows a triangular pulse. Both the square and triangular pulses become zero at $x = \pm a$. The pulses are plotted versus x/a and the transforms versus ka.

the transform, which we take to be the distance between the first zero-crossings on either side of $k = 0$, is $\Delta k = 2 \times \pi/a = 2\pi/a$. That is $\Delta x \Delta k = 2\pi$, which is independent of a.

Figure 5.5 also shows the shape and transform of a triangular pulse that goes to zero at $x = \pm a/2$. It is not hard to show that the Fourier Transform for this shape is $(8/ak^2)\sin^2(ak/4)$, which falls to zero more rapidly than for the square pulse. Once again, geometrically, we take $\Delta x = a$ and $\Delta k = 2 \times \pi/4a = \pi/2a$ so that $\Delta x \Delta k = \pi/2$. It seems that this pulse is "narrower" than the square pulse because $\Delta x \Delta k$ is smaller.

For homework, you will work out the Fourier Transform of a Gaussian pulse. In this case, you can actually calculate the widths. You will find that $\Delta x \Delta k$ is smaller still.

5.5.4 Working in k-space versus x-space

There is a good opportunity here to discuss quantum mechanics and electrical engineering, but I don't think there will be time.

5.6 The Dirac δ-function

Here's an interesting question: "What is the Fourier Transform of $f(x) = 1$?" This function is infinitely broad, so do we expect the Fourier Transform to be infinitely narrow? How would we quantify this?

Following (5.16) for $f(x) = 1$ leads us to

$$A(k) = \int_{-\infty}^{\infty} e^{-ikx}\, dx = \int_{-\infty}^{\infty} [\cos(kx) + i\sin(kx)]\, dx$$

The cosines and sines both give zero over any one period, so the integral is zero except for $k = 0$. In that case, we integrate unity over infinity and get infinity. That is, $A(k) = 0$ for $k \neq 0$ but is infinite when $k = 0$. That does sound like something that is infinitely narrow.

We can get more information by considering the integral of $A(k)$ about $k = 0$. Do this by integrating from $-\epsilon$ to $+\epsilon$ for some $\epsilon > 0$. Then

$$\begin{aligned}\int_{-\epsilon}^{\epsilon} A(k)dk &= \int_{-\epsilon}^{\epsilon} dk \int_{-\infty}^{\infty} e^{-ikx}\, dx = \int_{-\infty}^{\infty} dx \int_{-\epsilon}^{\epsilon} dk e^{-ikx} = \int_{-\infty}^{\infty} dx \frac{e^{-i\epsilon x} - e^{i\epsilon x}}{-ix} \\ &= 2\int_{-\infty}^{\infty} \frac{\sin(\epsilon x)}{x}\, dx = 2\int_{-\infty}^{\infty} \frac{\sin(y)}{y}\, dy = 4\int_{0}^{\infty} \frac{\sin(x)}{x}\, dx \qquad (5.19)\end{aligned}$$

where I made the substitution $y = \epsilon x$ in the second-to-last step, and finally recognized that the integral was symmetric about zero and switched the integration variable back to x.

The final integral in (5.19) can in fact be evaluated in several different ways. Here's one way, using a neat trick that seems to be attributed to the physicist Richard Feynman. The integral we need can be written as

$$I(0) = \int_0^{\infty} \frac{\sin(x)}{x}\, dx \qquad \text{where} \qquad I(s) = \int_0^{\infty} e^{-sx}\, \frac{\sin(x)}{x}\, dx$$

We don't know how to evaluate $I(s)$, but we can evaluate

$$\begin{aligned}I'(s) &= -\int_0^{\infty} e^{-sx}\, \sin(x)\, dx = -\frac{1}{2i}\int_0^{\infty} \left[e^{-sx+ix} - e^{-sx-ix}\right]\, dx \\ &= -\frac{1}{2i}\left[\frac{e^{-sx+ix}}{-s+i} - \frac{e^{-sx-ix}}{-s-i}\right]_0^{\infty} = \frac{1}{2i}\left[\frac{1}{-s+i} - \frac{1}{-s-i}\right] = -\frac{1}{1+s^2}\end{aligned}$$

Clearly $I(s) \to 0$ as $s \to \infty$, so

$$I(0) = -\int_0^{\infty} I'(s)\, ds = \int_0^{\infty} \frac{1}{1+s^2}\, ds = \tan^{-1}(s)\Big|_0^{\infty} = \frac{\pi}{2}$$

Therefore (5.19) becomes

$$\int_{-\epsilon}^{\epsilon} A(k)dk = 2\pi$$

Remarkably, we have been able to quantify the "infinity" at $k = 0$ for Fourier Transform of unity. Indeed, we write

$$\delta(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx}\, dx \tag{5.20}$$

in which case the Fourier Transform of unity is $A(k) = 2\pi\delta(k)$. The function $\delta(k)$ is called the *Dirac δ-function*. You will encounter this (very peculiar) function over and over in the course of studying physics.

Equation (5.20) is only one of very many representations of the Dirac δ-function. For our purposes, *it is sufficient to define $\delta(x)$ as a function which is zero for all $x \neq 0$, but it is "large enough" at $x = 0$ so that*

$$\int_{-\epsilon}^{\epsilon} \delta(x)\, dx = 1$$

for some $\epsilon > 0$. Some other representations for $\delta(x)$ might include a "box" of width a centered at $x = 0$ and with height $1/a$, or a Gaussian function normalized to have unit area in the limit of its width going to zero. The form (5.20) will be particularly useful in quantum mechanics.

A very useful property of the δ-function stems from the relation

$$\int_{-\epsilon}^{\epsilon} f(x)\delta(x)\, dx = f(0) \tag{5.21}$$

for some function $f(x)$. This is easy to see. Since ϵ can be taken as small as we want, it is essentially zero and we can take the $f(x = 0)$ out of the integral, leaving us only with the integral of $\delta(x)$.

There are also two-dimensional and three-dimensional versions of the δ-function, denoted as $\delta^{(2)}(\vec{r})$ and $\delta^{(3)}(\vec{r})$. It is straightforward to write these in Cartesian coordinates, for example $\delta^{(2)}(\vec{r}) = \delta(x)\delta(y)$, but more complicated in polar coordinates. However, it is simplest just to think of these in terms of the fundamental definition of the δ-function, that is $\delta^{(2)}(\vec{r})$ and $\delta^{(3)}(\vec{r})$ are zero for all $\vec{r}$ away from the origin, but

$$\int_S \delta^{(2)}(\vec{r})\, dS = 1 \qquad \text{and} \qquad \int_V \delta^{(3)}(\vec{r})\, dV = 1$$

for any surface S or volume V that encloses the origin.

5.6.1 Surface theorems revisited

We are now finally ready to resolve the apparent paradox we saw in Section 4.4. There was saw that the fields $\vec{B}(\vec{r})$ and $\vec{E}(\vec{r})$ given by (4.35) and (4.36) had zero curl and divergence, respectively, but the surface integrals in each case were nonzero. This seemed like a violation of Stokes' Theorem and Gauss' Theorem.

It is clear now, however, that there is one point, namely the origin, for which (4.35) and (4.36) are not really defined because the denominator goes to zero. Integrating over a surface or volume that encloses the origin gives a nonzero result because the curl and divergence are δ-functions at the origin. Indeed, for (4.35), we have

$$\vec{\nabla} \times \vec{B} = 2\pi a \, \delta^{(2)}(\vec{r}) \, \hat{k}$$

and for (4.36), we have

$$\vec{\nabla} \cdot \vec{E} = 4\pi a \, \delta^{(3)}(\vec{r})$$

In electromagnetism, $\vec{B}$ is the magnetic field from a long, straight, infinitely thin wire in the z-direction, and $\vec{E}$ is the electric field from a point charge.

5.7 Convolution

I won't be able to get to this.

5.8 Green's functions revisited

I won't be able to get to this either. Didn't manage to get to Green's Functions the first time around anyway!

Chapter 6

Vectors and Matrices

This chapter concerns the subject known as *Linear Algebra*. As with so many things in this course, this is a very large subject so we are only able to scratch the surface.

I will introduce the subject with a very specific example that I can use to set the stage, namely the problem of how to solve systems of linear algebraic equations. From there, I will get more formal and generalize to other kinds of physical systems.

6.1 Introduction to Systems of Linear Equations

How would you go about solving the system of equations

$$\begin{aligned} 2x + y &= 3 && \text{(6.1a)} \\ x - y &= 0 && \text{(6.1b)} \end{aligned}$$

for the variables x and y? A glance at the second equation tells you that $x = y$, and in your head you see that this gives $x = y = 1$ from the first equation. Of course, this is a very simple example, but you know that, in principle, you are able to multiply either or both of the equations by constants, add or subtract the equations from each other, and manipulate things one way or another so that you can isolate x and y.

Sometimes you encounter pitfalls, though. Consider solving the system of equations

$$\begin{aligned} 2x + y &= 3 && \text{(6.2a)} \\ 4x + 2y &= 6 && \text{(6.2b)} \end{aligned}$$

for x and y. If you multiply the first equation by 2 and subtract it from the second equation, you end up with $0 = 0$, which is true, but useless for finding x and y. (If the right hand side of the second equation was something other than 6, you wouldn't even end up with a true statement.) The problem, of course, is that these two equations are not *independent*. That is, they are really the same equation, because the coefficients of x and y in the second equation are both just the same factor, namely 2, of the coefficients in the first equation.

Our first job in this chapter is to formalize how we will write systems of linear equations, and this will lead us into a discussion of *vectors* and *matrices*. The concept of a "vector" will be a very expanded version of what we discussed in Section 4.1. Seeing this formalism will create some obvious questions regarding how we solve systems of linear equations, so we'll next address those questions before coming back to solving these systems in Section 6.3.9.

So let's think about a system of equations with more than just two variables x and y. Rather than run through the alphabet, let's say there are N equations for N variables x_1, x_2, $\ldots x_N$. We'll use an upper case "A" to denote the coefficients with appropriate subscripts, and write

$$\begin{array}{ccccccccccc} A_{11}x_1 & + & A_{12}x_2 & + & A_{13}x_3 & + & \cdots & + & A_{1N}x_N & = & c_1 \\ A_{21}x_1 & + & A_{22}x_2 & + & A_{23}x_3 & + & \cdots & + & A_{2N}x_N & = & c_2 \\ A_{31}x_1 & + & A_{32}x_2 & + & A_{33}x_3 & + & \cdots & + & A_{3N}x_N & = & c_3 \\ \vdots & & \vdots & & \vdots & & & & \vdots & & \vdots \\ A_{N1}x_1 & + & A_{N2}x_2 & + & A_{N3}x_3 & + & \cdots & + & A_{NN}x_N & = & c_N \end{array} \tag{6.3}$$

where the c_N are just the numbers on the right hand sides of the equations. These equations are the same as writing

$$\sum_{j=1}^{N} A_{ij}x_j = c_i$$

where $i = 1, 2, 3, \ldots, N$. Using our summation notation agreement, where any index repeated twice is automatically summed over, we get the compact form

$$A_{ij}x_j = c_i \tag{6.4}$$

which is exactly equivalent to (6.3).

An even more economical way to write (6.3) or (6.4), which in fact is profound, is

$$\underline{\underline{A}}\,\underline{x} = \underline{c} \tag{6.5}$$

where

$$\underline{\underline{A}} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots & A_{1N} \\ A_{21} & A_{22} & A_{23} & \cdots & A_{2N} \\ A_{31} & A_{32} & A_{33} & \cdots & A_{3N} \\ \vdots & \vdots & \vdots & & \vdots \\ A_{N1} & A_{N2} & A_{N3} & \cdots & A_{NN} \end{bmatrix} \qquad \underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_N \end{bmatrix} \qquad \text{and} \qquad \underline{c} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_N \end{bmatrix} \tag{6.6}$$

define the (square) *matrix* $\underline{\underline{A}}$ and the *column vectors* $\underline{x}$ and $\underline{c}$. You can now easily visualize the sum (6.4) by imagining taking the top row of $\underline{\underline{A}}$, matching it against the column $\underline{x}$, multiplying each element by each other one-by-one, adding this up and equating it to the first element of $\underline{c}$, that is c_1. Then repeat for the second row and equate to c_2 and so forth.

Please take note that the notation that I'm using, a double underline for a matrix and a single underline for a column vector, is not anyone's standard so far as I can tell. Different books

use different notations, and some simply let you figure out what things are from context. I am using this notation because I can easily write it on the board in class.

Clearly, one can define a matrix that is not square. A proper course in Linear Algebra will go through the properties of these kinds of matrices as well. In Physics, however, we rarely encounter matrices that are not square, so I just won't bother to go there.

Notice that our matrix notation (6.5) is easily generalized to products of matrices. That is, something like $\underline{\underline{A}}\,\underline{\underline{B}}$ has elements

$$\left[\underline{\underline{A}}\,\underline{\underline{B}}\right]_{ij} = \left(\sum_{k=1}^{N}\right) A_{ik}B_{kj}$$

where I put parenthesis around the summation only to warn you that I'm going to stop writing the summation symbol and resort to our summation convention instead.

The order in which you write matrices and vectors matters! You can talk about $\underline{\underline{A}}\,\underline{x}$ for an $N \times N$ matrix $\underline{\underline{A}}$ and N-dimensional column vector $\underline{x}$. but $\underline{x}\,\underline{\underline{A}}$ is nonsense. Also, $\underline{\underline{A}}\,\underline{\underline{B}}$ and $\underline{\underline{B}}\,\underline{\underline{A}}$ are both legal, if $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are both $N \times N$ matrices, but in general $\underline{\underline{A}}\,\underline{\underline{B}} \neq \underline{\underline{B}}\,\underline{\underline{A}}$.

There is a very special and important matrix called the *Identity Matrix* $\underline{\underline{I}}$. Its elements are all zero except for the diagonal elements, which are all unity. That is

$$\underline{\underline{I}} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix} \qquad \text{i.e.} \qquad \left[\underline{\underline{I}}\right]_{ij} = \delta_{ij} \tag{6.7}$$

It should be clear that $\underline{\underline{I}}\,\underline{x} = \underline{x}$ for any column vector $\underline{x}$, and $\underline{\underline{I}}\,\underline{\underline{A}} = \underline{\underline{A}}$ for any matrix $\underline{\underline{A}}$.

There is one more thing to show you about systems of linear equations before we jump off into the formalism of matrices, vectors, vector spaces, and operators.

In principle, for some matrix $\underline{\underline{A}}$ there can exist an *inverse matrix* $\underline{\underline{A}}^{-1}$ such that

$$\underline{\underline{A}}^{-1}\underline{\underline{A}} = \underline{\underline{I}} = \underline{\underline{A}}\underline{\underline{A}}^{-1} \tag{6.8}$$

Armed with the inverse matrix, we can immediately write down the solution for the x_i represented in (6.5) simply by multiplying both sides by $\underline{\underline{A}}^{-1}$. That is

$$\underline{x} = \underline{\underline{A}}^{-1}\underline{c}$$

This gives you a glimpse of the practical power of using matrices to solve systems of linear equations. The pitfalls I mentioned at the start of this section will correspond to circumstances under which the inverse does not exist for a particular matrix $\underline{\underline{A}}$.

From here we will talk about what we really mean by a *vector*, namely as an element of a *vector space*. An *operator* can act on a vector to turn it into a different vector. In most cases, we can *represent* a vector by a column vector, and an operator by a matrix, but there are a lot of blanks to fill in before we get into this in any level of detail.

6.2 Generalized Vectors

Section 4.1.4 gave you a hint that a "vector" is actually much more than a collection of two or three coordinates that specify the position in a plane or in space. In fact, a mathematical definition of a vector requires a good deal of sophistication in order to define a *vector space*. A *vector* is an element of a vector space.

I'm going to take a more practical approach here. For one thing, we don't have a lot of time and I'm afraid of getting some of you lost in the formalism if I tried. (Nevertheless, I urge you to take a math course in Linear Algebra at some point.) Secondly, and more importantly, I think it is better to take an incremental approach to abstract notion of vectors. By now you should be comfortable with the vector as a quantity in two-dimensional or three-dimensional space. The abstraction level I will take you to now, will be for an N-dimensional space with vectors that might contain complex numbers.

I refer you to Chapters 6 and 7 of Nearing's book "Mathematical Tools for Physics" for a nice Physics-friendly description of vector spaces, including operations on vectors and matrices.

6.2.1 The N-Dimensional complex vector

This is the entity that we will consider a "generalized vector" in this course. As I said, it is not as general as it could be, but will work for us.

A *vector* $\underline{v}$ is a collection of N (possibly) complex numbers v_1, v_2, ..., v_N. That is $\underline{v} \in \mathbb{C}^N$. If we want to write $\underline{v}$ in terms of its specific elements, we do so with a *column vector*, namely

$$\underline{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{bmatrix}$$

We refer to the individual v_i as *components* of the vector. The collection of all possible vectors forms a *vector space*.

It is also possible to represent a vector by its *transpose*, that is

$$\underline{v}^{\mathsf{T}} = \begin{bmatrix} v_1 & v_2 & \cdots & v_N \end{bmatrix}$$

which we also refer to as a *column vector*. We will in fact more often use the *Hermitian transpose*

$$\tilde{\underline{v}} = \underline{v^*}^{\mathsf{T}} = \begin{bmatrix} v_1^* & v_2^* & \cdots & v_N^* \end{bmatrix}$$

which is the transpose of the complex conjugates of the components of $\underline{v}$. Sometimes, especially in Quantum Mechanics, we refer to the space of Hermitian conjugate vectors as the *dual space*.

Multiplying a vector by a (complex) numbers means to multiply each component by that number, that is

$$c\underline{v} = \begin{bmatrix} cv_1 \\ cv_2 \\ \vdots \\ cv_N \end{bmatrix}$$

for some complex number c. Clearly, $c\underline{v}$ is a member of the vector space, assuming that $\underline{v}$ is a member.

Addition must be a property of a vector space. Two vectors $\underline{u}$ and $\underline{v}$ can be added by adding their components, that is

$$\underline{u} + \underline{v} = \begin{bmatrix} u_1 + v_1 \\ u_2 + v_2 \\ \vdots \\ u_N + v_N \end{bmatrix}$$

and the result is also clearly a member of the vector space. In fact, the actions of addition and multiplication mean that any linear combination of two vectors is a vector. That is

$$\underline{w} = a\underline{u} + b\underline{v}$$

is a member of the same vector space as $\underline{u}$ and $\underline{v}$ where a and b are complex numbers.

The vector space needs to have an *identity* element under addition. This is of course the vector $\underline{0}$ where all components are zero. Furthermore, each element of the vector space needs to have an inverse, that is, something to which it can be added giving the result $\underline{0}$. For a vector $\underline{v}$, the inverse is clearly $-\underline{v} = c\underline{v}$ where $c = -1$.

I remind you again that I am using a rather specific definition of a vector, much more general than the simple object in 2D or 3D real space, but less general than in fact is possible. I'll come back to this point in Section 6.2.5.

6.2.2 Inner product and norm

The *inner product* of two vectors $\underline{u}$ and $\underline{v}$ means to take the Hermitian conjugate of the first one and multiply it by the second one, in the sense that you are multiplying a column vector by a row vector as if they were matrices. That is, the inner product is

$$\langle u|v\rangle = \underline{\tilde{u}}\,\underline{v} = u_i^* v_i$$

where I have employed the summation notation. Clearly $\langle u|v\rangle = \langle v|u\rangle^*$.

It should be obvious to you that the inner (i.e. dot) product of two 3D (real) vectors $\vec{a}$ and $\vec{b}$ is completely consistent with this definition. Indeed, if the inner product of two vectors is zero, we say that they are *orthogonal*.

The inner product of a vector with itself gives the square of the *norm* of the vector, that is

$$\langle v|v\rangle = v_i^* v_i = \sum_{i=1}^{N} |v_i|^2$$

Don't be surprised if every now and then I slip up and refer to the *length* of a vector instead of the norm. This is an obvious throwback to the physical notion of a vector measuring the location of some object in three dimensional space.

6.2.3 Unit vectors

Unit vectors are vectors whose norm equals unity. A particularly useful set of unit vectors are those where one component equals one and all other components equal zero. We might denote these unit vectors as

$$\underline{e}_i = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}$$

where the "1" is in the ith row of the column vector. It is clear that any vector $\underline{v}$ can be written as a linear combination of the unit vectors. That is

$$\underline{v} = v_i \, \underline{e}_i$$

where, again, we invoke the summation convention. (I'll stop staying this at some point.) We might say something like "the vector space is spanned by the unit vectors" because we can construct any vector using them in this way.

We say that the unit vectors form a *basis* for the vector space.

6.2.4 Dyadics and tensors

How might you think about an object like $\underline{u}\,\tilde{\underline{v}}$, that is the "product" of a vector and its Hermitian conjugate, but in the "wrong" order? It seems reasonable to think about this sort of thing in terms of matrix multiplication, and write

$$\underline{u}\,\tilde{\underline{v}} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{bmatrix} \begin{bmatrix} v_1^* & v_2^* & \cdots & v_N^* \end{bmatrix} = \begin{bmatrix} u_1 v_1^* & u_1 v_2^* & \cdots & u_1 v_N^* \\ u_2 v_1^* & u_2 v_2^* & \cdots & u_2 v_N^* \\ \vdots & \vdots & \cdots & \vdots \\ u_N v_1^* & u_N v_2^* & \cdots & u_N v_N^* \end{bmatrix}$$

In other words, this "wrong" product is a matrix. This actually turns out to be a very useful construction for Physics, and you will see it in various courses. It is a good way to understand the moment of inertia of rigid bodies in classical mechanics, for example.

We call this kind of construction a *dyadic* or *dyad*. It is a special form of something called a *tensor*. We won't spend much time on the concept of tensors in this course, but you will encounter them elsewhere in your studies of Physics.

6.2.5 Functions can form a vector space

Even though we talked about the complex vector in Section 6.2.1 as our context for this course, I will take a moment to talk about an important generalization beyond that. I'm inspired to do this because of a question Jacob Shin asked in class about what I meant when I referred to "orthogonal functions."

Recall from Section 5.3.1 that we argued that any function $f(x)$ with periodicity defined by $f(x+a) = f(x)$ could be written as a linear combination of the functions $e^{2in\pi x/a}$ where n is some integer. If we replace the idea of "inner product" of two vectors by the integration of two functions over the relevant domain, that is for any two functions $g(x)$ and $h(x)$ we write

$$\langle g(x)|h(x)\rangle = \int_{-a/2}^{a/2} g^*(x)h(x)\,dx$$

then we have a well defined vector space. The functions $(1/a)e^{2in\pi x/a}$ where $n \in \mathbb{Z}$ are the unit vectors that form the basis for any function that is a member of the vector space. It is pretty easy to see that they have unit norm, and are orthogonal to each other.

Another, and perhaps more interesting, example concerns the Legendre Polynomials $P_\ell(x)$ from Section 3.6.4. Although we didn't prove it, the $P_\ell(x)$ obey an orthogonality relationship

$$\int_{-1}^{1} P_n(x)P_m(x)\,dx = \frac{2}{2n+1}\delta_{nm}$$

(I did not bother to take the complex conjugate because the Legendre Polynomials are real.) This means that we could argue, in exactly the same way we did for Fourier Series, that any polynomial defined over the range $-1 \le x \le 1$ can be written as a linear combination of the Legendre Polynomials. That is, the (appropriately normalized) $P_\ell(x)$ form the basis vectors for the vector space of polynomials.

You will encounter both of these examples when you study Quantum Mechanics.

6.3 Operations on Vectors: Matrices

If we were talking about vector spaces in the abstract, the next thing to talk about would be "operations" on vectors. An *operator* is an object which can transform a vector into

another vector. Abstract operators are critical in the formulation of Quantum Mechanics, for example.

In our context, however, we will be representing operators on vectors as matrices. See, for example, (6.5) where the matrix $\underline{\underline{A}}$ operates on a vector $\underline{x}$ and transforms it into a vector $\underline{c}$. This is how we will formalize operations on vectors.

Matrices and their actions on vectors arrive naturally in almost ever area of Physics. In fact, we've already seen in Section 3.7.1 how this works in the coupled simple harmonic oscillator, although I didn't really show you that we were working with matrices and vectors. Nevertheless, extending this discussion to N masses, and important problem in classical mechanics known as "N-body oscillations", will rely heavily on matrix and vector formalism.

A common use of operators with which you are already familiar are rotations in ordinary three-dimensional (or two-dimensional) space. A position vector pointed in any direction can be rotated into a vector in a different direction, and that operation is performed by multiplying a vector by a rotation matrix. In two dimensions, for example, the rotation of $\vec{r} = \hat{\imath}x + \hat{\jmath}y$ into a vector $\vec{r}' = \hat{\imath}x' + \hat{\jmath}y'$ through and angle ϕ corresponds to the equations

$$\begin{aligned} x' &= x\cos\phi + y\sin\phi \\ y' &= -x\sin\phi + y\cos\phi \end{aligned}$$

which we can write in our vector and matrix notation now as

$$\underline{r}' = \underline{\underline{D}}\,\underline{r}$$

where

$$\underline{r}' = \begin{bmatrix} x' \\ y' \end{bmatrix} \qquad \underline{\underline{D}} = \begin{bmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{bmatrix} \qquad \text{and} \qquad \underline{r} = \begin{bmatrix} x \\ y \end{bmatrix}$$

Furthermore, as I've already mentioned, Quantum Mechanics is formalized in terms of operators and (abstract) vectors, where these are "represented" by matrices and column vectors. Special Relativity is best formulated in terms of "four vectors" which represent "position" in spacetime, that is, a point in 3D space at a particular time, and "translating to a new reference frame" means to operate on a four vector with the matrix of the Lorentz Transformation.

So now let's gather up many of the things we've been saying, and formalize them a bit. Much of what follows will therefore be a repeat of things earlier in this chapter, but I thought it would be a good idea to collect things into the same place. There is a lot of terminology that goes along with matrix algebra, so I'm hoping this section will be a handy reference.

6.3.1 Matrices multiplying vectors

A matrix $\underline{\underline{A}}$ multiplies a vector $\underline{u}$ creating a new vector $\underline{v}$ as

$$\underline{\underline{A}}\,\underline{u} = \underline{v} \tag{6.9}$$

If the vectors have dimension N, then $\underline{\underline{A}}$ is an $N \times N$ *square matrix*. We write $\underline{\underline{A}}$ in terms of its *elements* as

$$\underline{\underline{A}} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots & A_{1N} \\ A_{21} & A_{22} & A_{23} & \cdots & A_{2N} \\ A_{31} & A_{32} & A_{33} & \cdots & A_{3N} \\ \vdots & \vdots & \vdots & & \vdots \\ A_{N1} & A_{N2} & A_{N3} & \cdots & A_{NN} \end{bmatrix} \tag{6.10}$$

Equation (6.9) actually represents the N equations

$$A_{ij} u_j = v_i$$

where each value of i is a different equation. In the context of operators, the matrix $\underline{\underline{A}}$ operates on the vector $\underline{u}$ giving the vector $\underline{v}$.

To pictorially understand the operation (6.9) we imagine that the first row of $\underline{\underline{A}}$ is pulled out of the matrix, turned upright to line up alongside the column vector $\underline{u}$, and then each element of the two columns multiplied by each other and added up.[1] This sum then is set equal to the first row of the new vector $\underline{v}$.

This is all perfectly consistent with a different multiplication operation, namely

$$\tilde{\underline{u}}\, \underline{\underline{A}} = \tilde{\underline{v}} \tag{6.11}$$

which is that a row vector can multiply a matrix giving a new row vector. By elements,

$$u_i^* A_{ij} = v_j^*$$

Here, pictorially, the row vector is tilted upright, lined up against the columns of the matrix one-by-one, multiplying each pair and adding them up, repeating for each column. It is fair to think of this as the operator represented by $\underline{\underline{A}}$ operating *to the left* on the row (or dual) vector $\tilde{\underline{u}}$. This concept will be found all through Quantum Mechanics.

Since we now think of $\underline{\underline{A}}\,\underline{v}$ as a new (column) vector, or $\tilde{\underline{u}}\,\underline{\underline{A}}$ as a new (row) vector, the quantity

$$\langle u|A|v\rangle \equiv \tilde{\underline{u}}\, \underline{\underline{A}}\, \underline{v} = u_i^* A_{ij} v_j \tag{6.12}$$

is well defined by the properties of the inner product. In fact, in Quantum Mechanics we refer to a quantity like this as a *matrix element*.

6.3.2 Matrices multiplying other matrices

If the equation $\underline{\underline{A}}\,\underline{u} = \underline{w}$ means that $\underline{w}$ is created by operating on $\underline{u}$ with $\underline{\underline{A}}$, but $\underline{u}$ was in fact created by the action of $\underline{\underline{B}}$ on a different vector $\underline{v}$, that is $\underline{u} = \underline{\underline{B}}\,\underline{v}$, then we would write

$$\underline{\underline{A}}\,\underline{\underline{B}}\,\underline{v} = \underline{w}$$

[1] Note how each instance of the repeated index j in this equation is adjacent to the other. We will see this again when we multiply matrices in Section 6.3.2.

which implies that we can create a new matrix $\underline{\underline{C}} = \underline{\underline{A}}\,\underline{\underline{B}}$ with elements

$$C_{ij} = A_{ik}B_{kj}$$

where we note the placement of the inner indices k and the outer indices i and j. Pictorially, this means we pick out the first row of $\underline{\underline{A}}$, tilt it upright and line it up against the first column of $\underline{\underline{B}}$, multiply the pairs and sum up the results, and this becomes the first element of $\underline{\underline{C}}$ in the upper left corner. Then repeat with the first row of $\underline{\underline{A}}$ and the *second* column of $\underline{\underline{B}}$ to get the second element in the first row of $\underline{\underline{C}}$. Repeat this for all the columns of $\underline{\underline{B}}$, and then again for the second row of $\underline{\underline{A}}$, and so forth.

There is no reason, a priori, that the vector you get from multiplying $\underline{\underline{B}}$ on $\underline{v}$ and then multiplying the result by $\underline{\underline{A}}$ should be the same as if you first multiply $\underline{v}$ by $\underline{\underline{A}}$ and then multiply the result by $\underline{\underline{B}}$. In other words, in general

$$\underline{\underline{A}}\,\underline{\underline{B}} \neq \underline{\underline{B}}\,\underline{\underline{A}}$$

We say that *matrix multiplication is not commutative*. There is a lot of physics in knowing whether or not certain matrices commute.

6.3.3 Symmetric and diagonal matrices

A matrix is called *symmetric* if the elements above the diagonal are equal, pairwise, to the elements below the diagonal, just by flipping indices. That is, a matrix $\underline{\underline{A}}$ is symmetric if its elements obey

$$A_{ij} = A_{ji}$$

We will see a cleaner definition of a symmetric matrix in Section 6.3.4.

Certain matrices are called *diagonal matrices* if the only non-zero elements are along the diagonal. For example

$$\underline{\underline{A}} = \begin{bmatrix} a^{(1)} & 0 & \cdots & 0 \\ 0 & a^{(2)} & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & a^{(N)} \end{bmatrix}$$

Or, in term of elements,

$$A_{ij} = a^{(i)}\delta_{ij} = a^{(j)}\delta_{ij}$$

where we are <u>not</u> invoking the summation notation because the first i (or j) is a superscript in parentheses. An important special case is the identity matrix $\underline{\underline{I}}$ with elements $I_{ij} = \delta_{ij}$.

Clearly, all diagonal matrices are symmetric, since $\delta_{ij} = \delta_{ji}$.

It is worth noting that all diagonal matrices commute with each other, and their product is also diagonal, with the diagonal elements of the product matrix just equal to the individual element products. That is, if $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are both diagonal, then

$$\left(\underline{\underline{A}}\,\underline{\underline{B}}\right)_{ij} = a^{(i)}\delta_{ik}b^{(j)}\delta_{kj} = a^{(i)}b^{(j)}\delta_{ij} = b^{(i)}a^{(j)}\delta_{ij} = b^{(i)}\delta_{ik}a^{(j)}\delta_{kj} = \left(\underline{\underline{B}}\,\underline{\underline{A}}\right)_{ij}$$

6.3.4 Transpose and Hermitian transpose of a matrix

The *transpose* $\underline{\underline{A}}^{\mathsf{T}}$ of a matrix $\underline{\underline{A}}$ has the same components as the original matrix but with its rows and columns reversed. That is, in terms of elements

$$\left(\underline{\underline{A}}^{\mathsf{T}}\right)_{ij} = \left(\underline{\underline{A}}\right)_{ji}$$

Clearly, a succinct definition of a symmetric matrix is just when a matrix equals its transpose. In other words, $\underline{\underline{A}}$ is a symmetric matrix if

$$\underline{\underline{A}}^{\mathsf{T}} = \underline{\underline{A}}$$

Given that our vectors and matrices are possibly made of complex numbers, we will find it handy to also define the *Hermitian transpose* which is the transpose of the complex conjugates of the elements of the original matrix, completely analogous to the situation with vectors. That is the Hermitian transpose[2] $\tilde{\underline{\underline{A}}}$ of a matrix $\underline{\underline{A}}$ has elements

$$\left(\tilde{\underline{\underline{A}}}\right)_{ij} = \left(\underline{\underline{A}}\right)^*_{ji}$$

If the Hermitian transpose leaves the matrix unchanged, we say the matrix is *Hermitian*. That is, $\underline{\underline{A}}$ is Hermitian if

$$\tilde{\underline{\underline{A}}} = \underline{\underline{A}}$$

It is easy to show that the transpose of a product of matrices is the product of the transposed matrices, but in the reverse order. That is

$$\left(\underline{\underline{A}}\,\underline{\underline{B}}\right)^{\mathsf{T}} = \underline{\underline{B}}^{\mathsf{T}}\underline{\underline{A}}^{\mathsf{T}} \tag{6.13}$$

Just write this out in terms of elements to prove the assertion. We have

$$\left[\left(\underline{\underline{A}}\,\underline{\underline{B}}\right)^{\mathsf{T}}\right]_{ij} = \left(\underline{\underline{A}}\,\underline{\underline{B}}\right)_{ji} = A_{jk}B_{ki} = \left(\underline{\underline{A}}^{\mathsf{T}}\right)_{kj}\left(\underline{\underline{B}}^{\mathsf{T}}\right)_{ik} = \left(\underline{\underline{B}}^{\mathsf{T}}\right)_{ik}\left(\underline{\underline{A}}^{\mathsf{T}}\right)_{kj} = \left(\underline{\underline{B}}^{\mathsf{T}}\underline{\underline{A}}^{\mathsf{T}}\right)_{ij}$$

Notice how I made use of the "adjacent indices" association with the matrix product by putting the two k indices next to each other in the second-to-last step.

It is straightforward to prove that the same thing holds for the Hermitian transpose. That is

$$\widetilde{\underline{\underline{A}}\,\underline{\underline{B}}} = \tilde{\underline{\underline{B}}}\,\tilde{\underline{\underline{A}}} \tag{6.14}$$

[2] If I were writing these notes to get students ready for Quantum Mechanics, I would have used the "dagger" notation instead of the "tilde" notation for dual vectors and Hermitian transpose matrices. That is, here I am writing $\tilde{\underline{\underline{A}}}$ instead of $\underline{\underline{A}}^{\dagger}$. However, these concepts are more generally useful and the only place I'm aware that "daggers" are used is in Quantum Mechanics.

6.3.5 Determinant of a matrix

The *determinant* $|\underline{\underline{A}}|$ of a matrix $\underline{\underline{A}}$ is an extremely important concept which unfortunately is difficult to clearly define.[3] Happily, we don't have to calculate the determinant often, and can generally leave that task to MATHEMATICA or some other application. I will nevertheless go through the basics here.

The determinant is a peculiar thing, mathematically. It maps the matrices, which we'd write as the Cartesian product $\mathbb{C}^N \times \mathbb{C}^N$ onto $\mathbb{C}$. That is, it takes a very large set and maps it into a much smaller set. (Never mind that both sets are actually infinite.)

Probably the best way to think about the determinant is as the sum of the N terms formed from every possible product of the elements of the matrix, picking from each row and one from each column, but never repeating the row or column, and including an alternating sign. You could write it as the sum over the products of all the elements but including an N-dimensional version of the totally antisymmetric symbol ϵ_{ijk} introduced in Section 4.1.2.

Let's use this to get the idea. if $\underline{\underline{A}}$ a 1×1 matrix then the determinant is just the single element A_{11}. For a 2×2 matrix, it's more complicated but still pretty simple. We just have to multiply along the left and right diagonals, and include the minus sign. That is

$$|\underline{\underline{A}}| = \begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix} = A_{11}A_{22} - A_{12}A_{21}$$

For a 3×3 matrix, it gets a little hairy, but let's take it slowly. Go across the top row, and with each element, form the product with the remaining rows and columns. There are two choices for each element in the top row. Remembering to alternate signs, you get

$$\begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = \begin{array}{r} A_{11}A_{22}A_{33} - A_{11}A_{23}A_{32} \\ -A_{12}A_{21}A_{33} + A_{12}A_{23}A_{31} \\ +A_{13}A_{21}A_{32} - A_{13}A_{22}A_{31} \end{array}$$

This determinant can be rewritten neatly in terms of 2×2 determinants as

$$\begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = A_{11} \begin{vmatrix} A_{22} & A_{23} \\ A_{32} & A_{33} \end{vmatrix} - A_{12} \begin{vmatrix} A_{21} & A_{23} \\ A_{31} & A_{33} \end{vmatrix} + A_{13} \begin{vmatrix} A_{21} & A_{22} \\ A_{31} & A_{32} \end{vmatrix}$$

It is easy to see that the three 2×2 matrices in this formula are obtained by removing from the original matrix the row and column corresponding to the top row element in question.

I won't prove it, but I think you can believe that this procedure extends to $N \times N$ matrices. That is, go along the top row (or any other row, for that matter), select the elements one by one, then multiply that element by the determinant of the sub-matrix obtained by removing the row and column of the element. This corresponding $(N-1) \times (N-1)$ determinant, along

[3] Never confuse $|\underline{\underline{A}}|$ with the concept of "absolute value". Sometimes we write $\det \underline{\underline{A}}$ for $|\underline{\underline{A}}|$.

with the appropriate sign, is called the *cofactor* of the element you selected. This procedure is called a *cofactor expansion* or *Laplace's expansion.*

This is enough to write down some important properties of determinants. I won't prove any of them, but hopefully they will seem at least plausible to you.

1. If you interchange any two rows or columns of a matrix, then the determinant changes sign. An obvious corollary is that the determinant $|\underline{\underline{A}}| = 0$ for any matrix $\underline{\underline{A}}$ that has two identical rows or columns.

2. If any one row or column of a matrix $\underline{\underline{A}}$ is multiplied by a constant c, then the determinant is $c|\underline{\underline{A}}|$. It therefore follows that if any one row (column) of a matrix is proportional to any other row (column), then $|\underline{\underline{A}}| = 0$.

3. If a matrix $\underline{\underline{A}}$ is multiplied by a constant c, then the determinant is multiplied by c^N, that is $|c\underline{\underline{A}}| = c^N|\underline{\underline{A}}|$.

4. The determinant of the transpose of a matrix is the same as the determinant of the original matrix, that is $|\underline{\underline{A}}^{\mathsf{T}}| = |\underline{\underline{A}}|$.

5. The determinant of the Hermitian transpose of a matrix equals the complex conjugate of the determinant of the original matrix, that is $|\underline{\underline{\tilde{A}}}| = |\underline{\underline{A}}|^*$.

6. For two matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$, $|\underline{\underline{A}}\,\underline{\underline{B}}| = |\underline{\underline{A}}||\underline{\underline{B}}| = |\underline{\underline{B}}\,\underline{\underline{A}}|$. That is, the determinant of the product of matrices is the product of the determinants, regardless of whether or not $\underline{\underline{A}}$ and $\underline{\underline{B}}$ commute.

We will rely on the properties of the determinant much more than actually calculating determinants. In any case, as I mentioned, nobody really calculates determinants anymore, much the same as that nobody calculates square roots anymore. We leave these to computer applications now.

The most important reason for us to know about the determinant is because it is needed to predict properties of matrix inversion. We take that up now.

6.3.6 Matrix inversion

Another important result that we are not going to prove, is that the elements of the inverse $\underline{\underline{A}}^{-1}$ of a matrix $\underline{\underline{A}}$ are given by

$$\left(\underline{\underline{A}}^{-1}\right)_{ij} = \frac{1}{|\underline{\underline{A}}|}\left(\underline{\underline{C}}^{\mathsf{T}}\right)_{ij} \tag{6.15}$$

where $\underline{\underline{C}}$ is the matrix of cofactors. That is, an element C_{ij} of $\underline{\underline{C}}$ is just the cofactor you get when you remove the ith row and jth column of $\underline{\underline{A}}$. As with the determinant, we rarely actually calculate the inverse matrix anymore, and leave that up to computer applications.

The important point from (6.15) is that if $|\underline{\underline{A}}| = 0$ then there is no inverse. As we mentioned in the properties of the determinant, this happens if any two rows or columns are identical, or if any row or column is just a factor times another row or column.

The inverse of a diagonal matrix is the diagonal matrix of the inverse of each of the diagonal elements in order. In addition to sounding like this makes sense, it is easy to show. Writing $A_{ij} = a^{(i)}\delta_{ij}$, then we are saying that $A^{-1}_{ij} = [1/a^{(i)}]\delta_{ij}$ so writing it out we get

$$\left(\underline{\underline{A}}^{-1}\underline{\underline{A}}\right)_{ij} = A^{-1}_{ik}A_{kj} = \frac{1}{a^{(i)}}\delta_{ik}\,a^{(j)}\delta_{kj} = \frac{a^{(j)}}{a^{(i)}}\delta_{ij} = \left(\underline{\underline{I}}\right)_{ij}$$

6.3.7 Orthogonal, Hermitian, and unitary matrices

This section is just to define three types of matrices. I will give you some indication of why they are important for different physical situations.

A matrix $\underline{\underline{A}}$ is said to be *orthogonal* if its transpose equals its inverse, that is $\underline{\underline{A}}^{\mathsf{T}} = \underline{\underline{A}}^{-1}$. The name comes from the fact that these matrices create rotations in two or three dimensions, and rotations maintain the orthogonality (and norm) of vectors. Note that the elements of such rotation matrices are real numbers, so there is no difference between the transpose and Hermitian transpose for rotation matrices.

Let's see how this works in the case of rotations in two dimensions. For a rotation through and angle ϕ, the inverse is simply obtained by taking $\phi \to -\phi$, so we have

$$\underline{\underline{A}} = \begin{bmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{bmatrix} \qquad \text{therefore} \qquad \underline{\underline{A}}^{-1} = \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix} = \underline{\underline{A}}^{\mathsf{T}}$$

(It is simple to prove this is the right inverse, just by multiplying out $\underline{\underline{A}}^{-1}\,\underline{\underline{A}}$.)

A *Hermitian matrix* is one for which the Hermitian transpose leaves it unchanged, that is $\underline{\underline{\tilde{A}}} = \underline{\underline{A}}$. In Quantum Mechanics, Hermitian matrices represent measurable quantities aka "observables." This is closely tied to the fact that Hermitian matrices have real eigenvalues, as we will discuss in Section 6.4.

If a matrix $\underline{\underline{U}}$ has the property that its Hermitian transpose equals its inverse, that is $\underline{\underline{\tilde{U}}} = \underline{\underline{U}}^{-1}$, then we say the matrix is *unitary*. Unitary matrices are practically useful for changing from one basis of a vector space to another. All real, orthogonal matrices are obviously unitary, and are, in fact, useful for changing the axes (i.e. "basis") for locations in two- or three-dimensional space.

6.3.8 Classifying matrices with groups

Will have to figure out how far I can go into this. Maybe just no time.

6.3.9 Revisiting systems of linear equations

We have now gone through all of the necessary material to justify the methodology outlined in Section 6.1 on solving systems of linear algebraic equations. I introduced the subject of Linear Algebra this way so that you could immediately see the practical importance of the formalism. This formalism is, however, useful for a very wide range of Physics problems. We will begin to see that now, as we study the formalism of eigenvalues and eigenvectors.

Maybe this is a good time to remind you that we've in fact already used this formalism in Section 3.1.1, where we came up with the Wronskian as defined in (3.5) to see if solutions to a linear ordinary differential equation were independent. The idea was that the ability to satisfy the boundary conditions on the function and its derivative(s) meant that we had to solve a system of linear equations. Linear independence meant that that system had to have a solution, which required the determinant of the coefficients, that is the Wronskian, to be nonzero.

6.4 The Eigenvalue Problem

A matrix $\underline{\underline{A}}$ operates on a vector $\underline{v}$ turning into another vector $\underline{u}$. Suppose (for reasons that will become clear shortly) we ask ourselves what it means if $\underline{u}$ is the same vector as $\underline{v}$, perhaps multiplied by some constant λ. That is

$$\underline{\underline{A}}\,\underline{v} = \lambda\,\underline{v} \tag{6.16}$$

In fact, this situation arises very often while solving problems in the physical sciences. We saw it, for example, in Section 3.7. (I'll be more explicit in Section 6.4.5.)

Equation (6.16) is called an *eigenvalue equation*. For a given matrix $\underline{\underline{A}}$, the constant λ is called an *eigenvalue* and the vector $\underline{v}$ is called an *eigenvector*.

Notice that I can multiply (6.16) through by a constant c, in which the eigenvector would be $c\underline{v}$, so there is clearly some freedom in choosing the norm of $\underline{v}$. In most problems, we agree that $\underline{v}$ should have unit norm, and that determines the value of $c = 1/\langle v|v\rangle^{1/2}$.

We will see that an $N \times N$ matrix has N eigenvalues and N eigenvectors to go with each of the eigenvalues. It is possible that two or more eigenvalues will be equal to each other, and that introduces some complications. These complications are easily overcome, but we won't bother with these situations in this course.

I will illustrate the fundamentals and usefulness of the eigenvalue problem by giving a specific example, namely finding the axes of a tilted ellipse. Along the way we'll prove a general theorem or two that help show why this is such and important problem. After the tilted ellipse, we'll get into the nitty gritty of how to solve the eigenvalue problem in general, that is, finding the eigenvalues and eigenvectors.

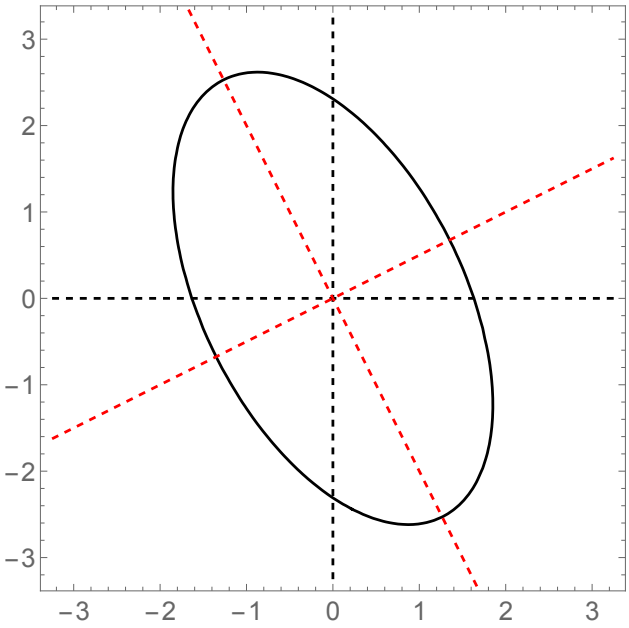


Figure 6.1: The black curve shows the "tilted ellipse" $6x^2+4xy+3y^2=16$. The object of this exercise is to find the directions of the major and minor axes of the ellipse, drawn here in red dashed lines. In fact, this problem is neatly solved using the eigenvalue approach, resulting in a transformation that "diagonalizes" the matrix used to write the left hand side of the equation. Details are in Section 6.4.1.

6.4.1 The axes of a tilted ellipse

Figure 6.1 plots the points which satisfy the equation

$$6x^2 + 4xy + 3y^2 = 16 \tag{6.17}$$

which you probably know is the equation of an ellipse. The presence of the "cross term" proportional to xy means that the ellipse is "tilted." That is, its axes do not line up with the x- and y-axes, as ellipses are usually drawn.

Our job is to find the directions of the axes (in red in Figure 6.1) along which the major and minor axes lie. We'll do this by looking for the rotation matrix $\underline{\underline{R}}$ that rotates the x- and y-axes into new axes x' and y' so that the cross terms in (6.17) vanish when written in terms of x' and y' instead of x and y.

The first step is to write (6.17) in terms of vectors and matrices. This is easy, that is

$$\underline{x}^{\mathsf{T}}\,\underline{\underline{A}}\,\underline{x} = 16 \qquad \text{where} \qquad \underline{\underline{A}} = \begin{bmatrix} 6 & 2 \\ 2 & 3 \end{bmatrix} \qquad \text{and} \qquad \underline{x} = \begin{bmatrix} x \\ y \end{bmatrix} \tag{6.18}$$

I am using the transpose instead of the Hermitian transpose because these are all real matrices, so that is simpler, and transpose and Hermitian transpose are therefore the same.

I had other choices for $\underline{\underline{A}}$, but I chose this form because it is a symmetric matrix. You'll see soon why that is the choice I had to make.

Now we are looking for the real, orthogonal matrix $\underline{\underline{R}}$ that makes the transformation $\underline{x} = \underline{\underline{R}}\,\underline{x}'$ which gets rid of the cross terms in the equation of the ellipse. (Technically, we are looking for the transformation that takes $\underline{x}$ to $\underline{x}'$, but that's just the inverse transformation, given

by the transpose of $\underline{\underline{R}}$.) Since the transformation equation implies that $\underline{x}^{\mathrm{T}} = (\underline{x}')^{\mathrm{T}}\underline{\underline{R}}^{\mathrm{T}}$, the ellipse equation (6.18) becomes

$$(\underline{x}')^{\mathrm{T}}\underline{\underline{R}}^{\mathrm{T}}\,\underline{\underline{A}}\,\underline{\underline{R}}\,\underline{x}' = 16 \tag{6.19}$$

There are no cross terms in (6.19) if the matrix $\underline{\underline{R}}^{\mathrm{T}}\,\underline{\underline{A}}\,\underline{\underline{R}}$ is diagonal. Therefore, our job reduces, mathematically, to finding the orthogonal matrix $\underline{\underline{R}}$ that "diagonalizes" the symmetric matrix $\underline{\underline{A}}$.

The eigenvalue problem solves this problem for us, because of a very important theorem that I will now state and prove. **The eigenvectors of a Hermitian matrix form an orthogonal set.** A byproduct of this proof will be a proof that the eigenvalues of a Hermitian matrix are real numbers.

The proof starts here. Consider two eigenvalues $\lambda^{(a)}$ and $\lambda^{(b)}$, and their corresponding eigenvectors $\underline{v}_a$ and $\underline{v}_b$. The eigenvalue equations are

$$\underline{\underline{A}}\,\underline{v}_a = \lambda^{(a)}\underline{v}_a \qquad \text{and} \qquad \underline{\underline{A}}\,\underline{v}_b = \lambda^{(b)}\underline{v}_b$$

Now take the inner product from the left with $\underline{v}_b$ on the first equation, and with $\underline{v}_a$ on the second equation. This gives

$$\tilde{\underline{v}}_b\,\underline{\underline{A}}\,\underline{v}_a = \lambda^{(a)}\tilde{\underline{v}}_b\,\underline{v}_a \qquad \text{and} \qquad \tilde{\underline{v}}_a\,\underline{\underline{A}}\,\underline{v}_b = \lambda^{(b)}\tilde{\underline{v}}_a\,\underline{v}_b \tag{6.20}$$

Now look at the left hand side of the first equation. This is a number that we can write as

$$\tilde{\underline{v}}_b\,\underline{\underline{A}}\,\underline{v}_a = v^*_{b_i}A_{ij}v_{a_j} = \left(v_{b_i}A^*_{ij}v^*_{a_j}\right)^* = \left(v^*_{a_j}\tilde{A}_{ji}v_{b_i}\right)^* = \left(\tilde{\underline{v}}_a\,\underline{\underline{\tilde{A}}}\,\underline{v}_b\right)^*$$

For the right side of the first equation, we have something similar, namely

$$\tilde{\underline{v}}_b\,\underline{v}_a = v^*_{b_i}v_{a_i} = \left(v_{b_i}v^*_{a_i}\right)^* = (\tilde{\underline{v}}_a\,\underline{v}_b)^*$$

In other words, flipping the order of these inner products means to take the complex conjugate of the result, and replacing the matrix by its Hermitian conjugate. This all means that we can rewrite (6.20) by using the above relationships and taking the complex conjugate of the first equation and get

$$\tilde{\underline{v}}_a\,\underline{\underline{\tilde{A}}}\,\underline{v}_b = \lambda^{(a)^*}\tilde{\underline{v}}_a\,\underline{v}_b \qquad \text{and} \qquad \tilde{\underline{v}}_a\,\underline{\underline{A}}\,\underline{v}_b = \lambda^{(b)}\tilde{\underline{v}}_a\,\underline{v}_b \tag{6.21}$$

If $\underline{\underline{A}}$ is Hermitian, that is $\underline{\underline{\tilde{A}}} = \underline{\underline{A}}$, then the left sides of these two equations are the same. Subtracting them tells us that

$$0 = \left(\lambda^{(a)^*} - \lambda^{(b)}\right)\tilde{\underline{v}}_a\,\underline{v}_b$$

Now if $a = b$, then the inner product $\tilde{\underline{v}}_a\,\underline{v}_b$ is positive definite, so

$$\lambda^{(a)^*} = \lambda^{(a)}$$

proving that the eigenvalues are real. On the other hand, if $a \neq b$, and the eigenvalues are distinct, then

$$\underline{\tilde{v}}_a \, \underline{v}_b = 0$$

and the eigenvectors are orthogonal. (As I mentioned earlier, I am leaving the case of different eigenvectors having the same eigenvalue to a more advanced course.) **This completes the proof.**

Now let's see how this helps us figure out the axes of a tilted ellipse. Our matrix $\underline{\underline{A}}$ is real and symmetric, so it is also Hermitian. Therefore, the two eigenvectors of $\underline{\underline{A}}$ will be orthogonal to each other.

This tells us how to build $\underline{\underline{R}}$. First remember that since $\underline{\underline{R}}$ is an orthogonal matrix, $\underline{\underline{R}}^{\mathsf{T}} \underline{\underline{R}} = \underline{\underline{I}}$. Now, build $\underline{\underline{R}}$ by making its columns equal to the (normalized) eigenvectors of $\underline{\underline{A}}$. When we do $\underline{\underline{A}}\,\underline{\underline{R}}$, then, each column will be just multiplied by the eigenvalue. So, when we do $\underline{\underline{R}}^{\mathsf{T}}$ on this, we will get a diagonal matrix with the eigenvalues along the diagonal! This is a general argument that will work any $N \times N$ matrix $\underline{\underline{A}}$.

This is all best illustrated by going back to our tilted ellipse problem. After doing the work to get the eigenvalues and eigenvectors of $\underline{\underline{A}}$ in (6.18), a procedure we will describe in detail in Section 6.4.2, we end up with eigenvalues

$$\lambda^{(1)} = 7 \qquad \text{and} \qquad \lambda^{(2)} = 2$$

corresponding to the (normalized) eigenvectors

$$\underline{v}_1 = \begin{bmatrix} 2/\sqrt{5} \\ 1/\sqrt{5} \end{bmatrix} \qquad \text{and} \qquad \underline{v}_2 = \begin{bmatrix} -1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix}$$

Using the eigenvectors as columns in the rotation matrix gives

$$\underline{\underline{R}} = \begin{bmatrix} 2/\sqrt{5} & -1/\sqrt{5} \\ 1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix} \qquad \text{and, so} \qquad \underline{\underline{R}}^{\mathsf{T}} = \begin{bmatrix} 2/\sqrt{5} & 1/\sqrt{5} \\ -1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix}$$

It is worth showing explicitly that $\underline{\underline{R}}$ is orthogonal, so let's do it.

$$\begin{aligned} \underline{\underline{R}}^{\mathsf{T}} \underline{\underline{R}} &= \begin{bmatrix} 2/\sqrt{5} & 1/\sqrt{5} \\ -1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix} \begin{bmatrix} 2/\sqrt{5} & -1/\sqrt{5} \\ 1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix} \\ &= \begin{bmatrix} 4/5 + 1/5 & -2/5 + 2/5 \\ -2/5 + 1/5 & 1/5 + 4/5 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \underline{\underline{I}} \end{aligned}$$

You should take a moment to convince yourself that $\underline{\underline{R}}\,\underline{\underline{R}}^{\mathsf{T}} = \underline{\underline{I}}$ as well.

Now let's check our conjecture that building $\underline{\underline{R}}$ this way "diagonalizes" the matrix $\underline{\underline{A}}$. We'll do this in two steps for the sake of illustration. First we multiply $\underline{\underline{A}}$ times $\underline{\underline{R}}$, so

$$\underline{\underline{A}}\,\underline{\underline{R}} = \begin{bmatrix} 6 & 2 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} 2/\sqrt{5} & -1/\sqrt{5} \\ 1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix} = \begin{bmatrix} 14/\sqrt{5} & -2/\sqrt{5} \\ 7/\sqrt{5} & 4/\sqrt{5} \end{bmatrix}$$

As predicted, this just multiplies each column by its respective eigenvalue. Of course, it had to be, because we built $\underline{\underline{R}}$ with columns that in fact were the eigenvectors of $\underline{\underline{A}}$.

Second, we complete the transformation indicated in (6.19) to get

$$\underline{\underline{R}}^{\mathsf{T}}\,\underline{\underline{A}}\,\underline{\underline{R}} = \begin{bmatrix} 2/\sqrt{5} & 1/\sqrt{5} \\ -1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix} \begin{bmatrix} 14/\sqrt{5} & -2/\sqrt{5} \\ 7/\sqrt{5} & 4/\sqrt{5} \end{bmatrix} = \begin{bmatrix} (28+7)/5 & (-4+4)/5 \\ (-14+14)/5 & (2+8)/5 \end{bmatrix} = \begin{bmatrix} 7 & 0 \\ 0 & 2 \end{bmatrix}$$

and, again as predicted, the transformed matrix is diagonal with elements given by the eigenvalues. Therefore, writing out (6.19) in terms of our tilted x'- and y'-axes,

$$7x'^2 + 2y'^2 = 16$$

which is the form we were aiming to achieve.

If we want to find the actual rotation angle that we used, just interpret the element R_{11} as the cosine of the angle. That is

$$\phi = \cos^{-1}\frac{2}{\sqrt{5}} = 26.6^\circ$$

To draw the red lines in Figure 6.1 we use the eigenvectors themselves. The eigenvectors point in the directions of the axes. The equation of a line through the origin is $\hat{n}\cdot\vec{r}$ where $\vec{r} = \hat{\imath}x + \hat{\jmath}y$ and $\hat{n}$ is a (unit) vector perpendicular to the line. Since the eigenvectors are orthogonal to each other, we use one eigenvector for the other axis. Therefore (multiplying through by $\sqrt{5}$) the equations of the red lines are

$$2x + y = 0 \qquad \text{and} \qquad -x + 2y = 0$$

To summarize, after proving a theorem about the eigenvectors of Hermitian matrices, we used the results of that theorem to build an orthogonal matrix $\underline{\underline{R}}$ that "diagonalized" the matrix $\underline{\underline{A}}$ which solved our problem of finding the tilted axes of an ellipse. It should be clear, however, that this approach would work for *any* $N \times N$ Hermitian (or real symmetric) matrix $\underline{\underline{A}}$. This touches on very many important physical problems.

Now that we see how this works, let's discuss how to actually go about finding the eigenvectors and eigenvalues of a matrix.

6.4.2 Finding eigenvalues and eigenvectors

First, I will own up to the fact that to find the eigenvalues and eigenvectors of the matrix $\underline{\underline{A}}$ in (6.18), I used the Eigensystem function in MATHEMATICA. Just as "nobody" calculates determinants anymore, "nobody" does the eigenvector calculation by hand. Nevertheless, we'll go through the procedure, just to show you that it is not magic. We'll also illustrate it with our 2×2 matrix example.

We first rewrite (6.16) slightly as

$$\underline{\underline{A}}\,\underline{v} = \lambda\,\underline{\underline{I}}\,\underline{v}$$

where we have inserted the identity matrix in front of $\underline{v}$, that is we've used $\underline{\underline{I}}\,\underline{v} = \underline{v}$. With a little bit of rearranging, this gives

$$\left(\underline{\underline{A}} - \lambda\,\underline{\underline{I}}\right)\underline{v} = \underline{0} \tag{6.22}$$

where we are being explicit that the right side of the equation is the column vector with all entries equal to zero. This is just a system of linear algebraic equations for the components of $\underline{v}$. What's more, it is a *homogeneous* system of equations. That means that we expect all of the components of $\underline{v}$ to be zero.

This is unacceptable, of course, so we need to prevent (6.22) from having a solution. We know how to do this, though. We just require that the determinant of the matrix on the left be zero. Mathematically, this means

$$\det\left(\underline{\underline{A}} - \lambda\,\underline{\underline{I}}\right) = \begin{vmatrix} A_{11}-\lambda & A_{12} & A_{13} & \cdots & A_{1N} \\ A_{21} & A_{22}-\lambda & A_{23} & \cdots & A_{2N} \\ A_{31} & A_{32} & A_{33}-\lambda & \cdots & A_{3N} \\ \vdots & \vdots & \vdots & & \vdots \\ A_{N1} & A_{N2} & A_{N3} & \cdots & A_{NN}-\lambda \end{vmatrix} = 0 \tag{6.23}$$

which is a polynomial of degree N in λ. This is called the *characteristic equation* and will have N roots. That is, it yields N values for λ.

Each value of λ makes (6.22) a different set of equations that can be solved for the components of $\underline{v}$. This system is no longer N independent equations, though, so the best you can do is to solve for $N-1$ components in terms of the one remaining. That's OK, though, because you want to normalize $\underline{v}$, giving you an additional equation, namely $\langle v|v\rangle = 1$.

It's best to illustrate this with a specific example, so let's use the matrix $\underline{\underline{A}}$ from (6.18). The characteristic equation is

$$\begin{vmatrix} 6-\lambda & 2 \\ 2 & 3-\lambda \end{vmatrix} = (6-\lambda)(3-\lambda) - 4 = \lambda^2 - 9\lambda + 14 = (\lambda-7)(\lambda-2) = 0$$

so the eigenvalues are indeed 7 and 2. For $\lambda = 7$, the system of equations is

$$\begin{aligned} -v_1 + 2v_2 &= 0 \\ 2v_1 - 4v_2 &= 0 \end{aligned}$$

which are indeed the same equation, which reduces to $v_1 = 2v_2$. Combining this with

$$\langle v|v\rangle = v_1^2 + v_2^2 = 5v_2^2 = 1$$

gives us $v_1 = 2/\sqrt{5}$ and $v_2 = 1/\sqrt{5}$ which is what we quoted for the eigenvector $\underline{v}$ corresponding to the eigenvalue $\lambda = 7$.For $\lambda = 2$, the system of equations is

$$\begin{aligned} 4v_1 + 2v_2 &= 0 \\ 2v_1 + v_2 &= 0 \end{aligned}$$

so $v_2 = -2v_1$ and so forth.

6.4.3 Coupled oscillations revisited

We studied the problem of two masses and three springs in Section 3.7.1. In fact, that is an ideal example of an eigenvalue problem in Physics, although we didn't call it that at a time. Formulating that problem in terms of eigenvectors is elegant, and straightforward to generalize to N masses.

In this section we will reformulate the problem of two identical masses connected by three identical springs in terms of vectors, matrices, and eigenvalues. First let's rewrite the coupled differential equations (3.31) as

$$\ddot{x}_1(t) = -2\omega_0^2 x_1(t) + \omega_0^2 x_2(t) \tag{6.24a}$$

$$\ddot{x}_2(t) = \omega_0^2 x_1(t) - 2\omega_0^2 x_2(t) \tag{6.24b}$$

In terms of vectors and matrices, we can write this as

$$\ddot{\underline{x}}(t) = -\omega_0^2 \, \underline{\underline{\Omega}} \, \underline{x}(t) \tag{6.25}$$

where we have made the definitions

$$\underline{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \text{and} \qquad \underline{\underline{\Omega}} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

It should be clear that if the masses and springs were not all the same, then the formulation would look the same, but the matrix $\underline{\underline{\Omega}}$ would be different.

Now we make our standard ansatz, which now takes the form

$$\underline{x}(t) = \underline{a}\, e^{i\omega t} \qquad \text{where} \qquad \underline{a} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \tag{6.26}$$

is a vector of constants a_1 and a_2. Taking the time derivative and dividing out the factor $e^{i\omega t}$ on both sides, the vector differential equation (6.25) now takes the form

$$\underline{\underline{\Omega}} \, \underline{a} = \lambda \underline{a} \qquad \text{where} \qquad \lambda = \frac{\omega^2}{\omega_0^2} \tag{6.27}$$

and we have arrived at an eigenvalue problem.

The eigenvalues of $\underline{\underline{\Omega}}$ are easy to determine. The characteristic equation is

$$\begin{vmatrix} 2-\lambda & -1 \\ -1 & 2-\lambda \end{vmatrix} = (2-\lambda)^2 - 1 = 0$$

is easily solved since $2 - \lambda = \pm 1$ so $\lambda = 1$ or $\lambda = 3$. As expected an $N \times N = 2 \times 2$ matrix has $N = 2$ eigenvalues. The eigenvectors are simple to find. Let's use a labeling scheme where the first eigenvalue is $\lambda = 1$, and the second eigenvalue is $\lambda = 3$. Then for $\lambda = 1$,

$$\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} a_1^{(1)} \\ a_2^{(1)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

which gives two equivalent equations for $a_1^{(1)}$ and $a_2^{(1)}$, namely $a_1^{(1)} - a_2^{(1)} = 0$ or $a_1^{(1)} = a_2^{(1)}$. Therefore, including a normalization, the first eigenvector is

$$\underline{a}^{(1)} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} \tag{6.28}$$

For the second eigenvalue $\lambda = 3$, we find the eigenvector using

$$\begin{bmatrix} -1 & -1 \\ -1 & -1 \end{bmatrix} \begin{bmatrix} a_1^{(2)} \\ a_2^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

which implies that $a_1^{(2)} + a_2^{(2)} = 0$, so the normalized eigenvector is

$$\underline{a}^{(2)} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix} \tag{6.29}$$

Of course, our real goal here is to find the motions of the two masses, that is $x_1(t)$ and $x_2(t)$, or, equivalently (and more succinctly) the vector $\underline{x}(t)$. Writing the solution as the ansatz (6.26) was just a means to a solution. What we have learned is that there are two solutions, one with "eigenfrequency" $\omega = \pm\omega_0 \equiv \pm\omega^{(1)}$ and the other with eigenfrequency $\omega = \pm\omega_0\sqrt{3} \equiv \omega^{(2)}$. The "$\pm$" is an artifact of our solving a second order differential equation, giving us in fact two solutions for each eigenvalue.

So, the general solution for the motion of the two masses is

$$\underline{x}(t) = c_+^{(1)}\underline{a}^{(1)}e^{i\omega^{(1)}t} + c_-^{(1)}\underline{a}^{(1)}e^{-i\omega^{(1)}t} + c_+^{(2)}\underline{a}^{(2)}e^{i\omega^{(2)}t} + c_-^{(2)}\underline{a}^{(2)}e^{-i\omega^{(2)}t} \tag{6.30}$$

where the four constants $c_+^{(1)}$, $c_-^{(1)}$, $c_+^{(2)}$, and $c_-^{(2)}$ are determined from the four initial conditions, namely the initial positions and velocities of each of the two masses. Look back now at (3.33), and refer to the eigenvectors $\underline{a}^{(1)}$ (6.28)and $\underline{a}^{(2)}$ (6.29). Equation (6.30) is the same as (3.33), where

$$\frac{1}{\sqrt{2}}c_+^{(1)} = a \qquad \frac{1}{\sqrt{2}}c_-^{(1)} = b \qquad \frac{1}{\sqrt{2}}c_+^{(2)} = c \qquad \frac{1}{\sqrt{2}}c_-^{(2)} = d$$

Let's continue with our vector and matrix notation and put in the initial conditions. The initial position and velocity vectors are

$$\underline{x}_0 = \begin{bmatrix} x_{1_0} \\ x_{2_0} \end{bmatrix} \qquad \text{and} \qquad \underline{v}_0 = \begin{bmatrix} v_{1_0} \\ v_{2_0} \end{bmatrix}$$

so applying (6.30) gives us

$$\begin{aligned} \underline{x}_0 &= c_+^{(1)}\underline{a}^{(1)} + c_-^{(1)}\underline{a}^{(1)} + c_+^{(2)}\underline{a}^{(2)} + c_-^{(2)}\underline{a}^{(1)} \\ &= \left[c_+^{(1)} + c_-^{(1)}\right]\underline{a}^{(1)} + \left[c_+^{(2)} + c_-^{(2)}\right]\underline{a}^{(2)} \\ \text{and} \qquad \underline{v}_0 &= i\omega^{(1)}c_+^{(1)}\underline{a}^{(1)} - i\omega^{(1)}c_-^{(1)}\underline{a}^{(1)} + i\omega^{(2)}c_+^{(2)}\underline{a}^{(2)} - i\omega^{(2)}c_-^{(2)}\underline{a}^{(1)} \\ &= i\omega^{(1)}\left[c_+^{(1)} - c_-^{(1)}\right]\underline{a}^{(1)} + i\omega^{(2)}\left[c_+^{(2)} - c_-^{(2)}\right]\underline{a}^{(2)} \end{aligned}$$

These equations look messy, but don't let that slow you down. Remember that the $\omega^{(1)}$ and $\omega^{(2)}$ are just numbers, as are the components of $\underline{x}_0$ and $\underline{v}_0$, so this is just four equations to solve for the $c_\pm^{(1)}$ and $c_\pm^{(2)}$ in terms of the other stuff.

If we look at a simple special case, we can get a better feeling for how the motion breaks down in terms of the eigenvectors. Let's say the two masses start from rest, that is $\underline{v}_0 = \underline{0}$. This means that $c_+^{(1)} = c_-^{(1)} \equiv c^{(1)}/2$ and $c_+^{(2)} = c_-^{(2)} \equiv c^{(2)}/2$, and

$$\underline{x}_0 = c^{(1)}\underline{a}^{(1)} + c^{(2)}\underline{a}^{(2)} \tag{6.31}$$

It is now clear how we excite the "eigenmodes." If we set $x_{1_0} = x_{2_0} = c$, that is

$$\underline{x}_0^{(1)} = \begin{bmatrix} c \\ c \end{bmatrix} = c\sqrt{2}\,\underline{a}^{(1)}$$

which just means that the initial positions of the two masses correspond to the eigenvalue $\lambda^{(1)} = 1$, i.e. $\omega = \omega_0$, then $c^{(2)} = 0$ in order to satisfy (6.31) and the motion (6.30) becomes

$$\underline{x}^{(1)}(t) = \frac{1}{2}c^{(1)}\underline{a}^{(1)}e^{i\omega^{(1)}t} + \frac{1}{2}c^{(1)}\underline{a}^{(1)}e^{-i\omega^{(1)}t} = c^{(1)}\underline{a}^{(1)}\cos\omega^{(1)}t = c\sqrt{2}\underline{a}^{(1)}\cos\omega_0 t$$

If we write this as two separate equations using the eigenvector $\underline{a}^{(1)}$ from (6.28), we have

$$x_1^{(1)}(t) = c\cos\omega_0 t \qquad \text{and} \qquad x_2^{(1)}(t) = c\cos\omega_0 t$$

In other words, in "eigenmode (1)", the two masses oscillate together, in phase, exactly as shown on the left in Figure 3.13.

To excite "eigenmode (2)", we set initial conditions that correspond to eigenvector $\underline{a}^{(2)}$ from (6.29). By setting $x_{1_0} = c$ and $x_{2_0} = c$ we have

$$\underline{x}_0^{(2)} = \begin{bmatrix} c \\ -c \end{bmatrix} = c\sqrt{2}\,\underline{a}^{(2)}$$

corresponding to $\lambda^{(2)} = 3$, i.e. $\omega = \omega_0\sqrt{3}$. We therefore set $c^{(1)} = 0$ in order to satisfy (6.31) and the motion (6.30) becomes

$$\underline{x}^{(2)}(t) = \frac{1}{2}c^{(2)}\underline{a}^{(2)}e^{i\omega^{(2)}t} + \frac{1}{2}c^{(2)}\underline{a}^{(2)}e^{-i\omega^{(2)}t} = c^{(2)}\underline{a}^{(2)}\cos\omega^{(2)}t = c\sqrt{2}\underline{a}^{(2)}\cos\omega_0\sqrt{3}t$$

Written as two separate equations using the eigenvector $\underline{a}^{(2)}$ from (6.29), we have

$$x_1^{(2)}(t) = c\cos\omega_0\sqrt{3}t \qquad \text{and} \qquad x_2^{(1)}(t) = -c\cos\omega_0\sqrt{3}t$$

In other words, in "eigenmode (2)", the two masses oscillate against each other, 180° out of phase, with a frequency that is $\sqrt{3}$ higher than for eigenmode (1), exactly as shown on the right in Figure 3.13.

To summarize, we have solved the problem of two identical masses connected the three identical springs using the eigenvalue problem formalism, and the result is (of course!) exactly the same as what we got with our seat-of-the-pants approach in Section 3.7.1.

The eigenvalue problem approach gets a little tedious when we actually get down to writing the motions of the two masses, but there is a very important reason why this approach is the better way to go. The differential equation written as (6.25) is much more elegant than writing the two separate equations (3.31), and it is much more easily generalized to systems of different masses or larger numbers of masses. In fact, in most physical problems, it isn't the actual motion of the individual masses that matter, but what are their eigenmodes and eigenfrequencies. This comes directly from constructing the $N \times N$ matrix $\underline{\underline{\Omega}}$ for a given problem with N masses.

6.4.4 Example: Principle axes of a rotating rigid body

This will be left to a MATHEMATICA lab.

6.4.5 Example: N-body oscillations

This will be left to a second semester mechanics course.

6.5 Four-Vectors in Spacetime

Not sure how much Special Relativity I can work in here. Would be great if I could work through boosts in the z-direction.

6.6 The Structure of Quantum Mechanics

Probably won't have time to cover any of this. Maybe just show them the notation to whet their appetite, refer to Townsend and MQM3e for details.

Chapter 7

Calculus of Variations

Here's a general mathematical problem that turns out to be very important in lots of scientific fields. Imagine you are looking to find some function $f(x)$ that is defined over a range $a \leq x \leq b$. You don't know much about the function, except that you have its values $f(a)$ and $f(b)$, and that there's an integral over this range that, involving this function, and you want that integral to be a minimum. In other words, you want to find the function $f(x)$ so that the integral

$$S = \int_a^b F\left[f(x), f'(x), x\right] dx \tag{7.1}$$

is minimized, where $f(a)$ and $f(b)$ have fixed values. You are given the function F of $f(x)$ and its derivatives (and perhaps x as well). How would you go about finding $f(x)$?

The solution to this general problem leads us into the *Calculus of Variations*. The first place you will encounter this problem in a Physics course will probably be Analytical Mechanics. You'll see that it is much more useful in general, though, and we'll do some examples before we're done with this chapter. There are also some fundamental physics implications, because lots of basic physical laws come down to minimizing the "action" over some "path" through space and time.

Sometimes the integral S in (7.1) is written as $S[f(x)]$. That is, S takes on a different value for a different function $f(x)$. We refer to $S[f(x)]$ by saying the S is a *functional* of $f(x)$.

You might be interested to know that although it took Einstein a decade to come up with the correct equations for General Relativity, the mathematician David Hilbert figured out how to do it with an action principle and came close to beating Einstein to the punch.[1]

We'll start this chapter by doing a specific example, namely showing that the shortest distance between two points is a straight line. Then we'll generalize the technique and do some examples.

[1] "A comment on the relations between Einstein and Hilbert", Heinrich Medicus, Am. J. Phys. 52(1984)206.

7.1 The Shortest Distance Between Two Points

What curve has the shortest distance between two points in a plane? Obviously, the answer is a straight line, but how would you go about proving that? Well, if you put the two points in the (x, y) plane and assume they are joined by a function $y = f(x)$, then you would integrate the length along this curve and look for the $f(x)$ that gives you the smallest value. The length of an infinitesimal area element in the (x, y) plane is

$$ds = \sqrt{dx^2 + dy^2}$$

Therefore, the length S between two points a and b in the (x, y) plane is

$$S = \int_a^b ds = \int_a^b \sqrt{dx^2 + dy^2} = \int_a^b \sqrt{1 + \left(\frac{dy}{dx}\right)^2}\, dx = \int_a^b \sqrt{1 + (f'(x))^2}\, dx \tag{7.2}$$

and we aim to find the function $y = f(x)$ that minimizes $S[f(x)]$. If we write

$$Y(x) = f(x) + \epsilon\eta(x)$$

where ϵ is just some parameter, $f(x)$ is the right function, and $\eta(x)$ is some arbitrary function, then maybe we can find $f(x)$ by considering $S[Y(x)] = S(\epsilon)$ and setting $dS/d\epsilon = 0$ when $\epsilon = 0$. Following our nose and using integration by parts, we have

$$\begin{aligned}
\frac{d}{d\epsilon}S(\epsilon) &= \frac{d}{d\epsilon}\int_a^b \sqrt{1 + (Y'(x))^2}\, dx = \int_a^b \frac{Y'(x)}{\sqrt{1 + (Y'(x))^2}}\frac{dY'}{d\epsilon}\, dx \\
\left.\frac{d}{d\epsilon}S(\epsilon)\right|_{\epsilon=0} &= \int_a^b \frac{f'(x)}{\sqrt{1 + (f'(x))^2}}\eta'(x)\, dx \\
&= \left.\frac{f'(x)}{\sqrt{1 + (f'(x))^2}}\eta(x)\right|_a^b - \int_a^b \frac{d}{dx}\left[\frac{f'(x)}{\sqrt{1 + (f'(x))^2}}\right]\eta(x)\, dx = 0
\end{aligned}$$

Now $\eta(x)$ is an arbitrary function, except that we require $\eta(a) = \eta(b) = 0$ so that $Y(x)$ has the right values at $x = a$ and $x = b$. So, the first term above is zero, and we are left with

$$\int_a^b \frac{d}{dx}\left[\frac{f'(x)}{\sqrt{1 + (f'(x))^2}}\right]\eta(x)\, dx = 0$$

This is in fact an interesting result. It says that the integral is zero no matter what function I choose for $\eta(x)$. The only way to achieve this is to have the factor multiplying $\eta(x)$ be zero. That is

$$\frac{d}{dx}\left[\frac{f'(x)}{\sqrt{1 + (f'(x))^2}}\right] = 0 \qquad \text{or} \qquad \frac{f'(x)}{\sqrt{1 + (f'(x))^2}} = \text{constant} \tag{7.3}$$

which is of course equivalent to $f'(x)$ =constant. In other words, the curve that connects $x = a$ to $x = b$ over the shortest distance is the one a constant slope, which is a straight line. We have proved our assertion.

7.2 The Euler-Lagrange Equations

The approach used to find the path with the shortest distance between two points, used in Section 7.1, can easily be generalized to find a condition on the function $F\left[f(x), f'(x), x\right]$ in (7.1) that minimizes the functional $S[f(x)]$.

We start the same way, and write

$$Y(x) = f(x) + \epsilon\eta(x) \qquad \text{with} \qquad \eta(a) = 0 = \eta(b)$$

where $f(x)$ is the correct answer and $\eta(x)$ is otherwise arbitrary. Whereas in Section 7.1 the integrand only depended on $f'(x)$, this time we have the integrand depending, in principle on $f(x)$ as well. Therefore, using the chain rule for a multivariable function,

$$\frac{d}{d\epsilon}S(\epsilon) = \int_a^b \left[\frac{\partial F}{\partial Y}\frac{\partial Y}{\partial \epsilon} + \frac{\partial F}{\partial Y'}\frac{\partial Y'}{\partial \epsilon}\right] dx$$

and the condition that $f(x)$ minimize $S(0)$ becomes

$$\frac{d}{d\epsilon}S(\epsilon)\bigg|_{\epsilon=0} = \int_a^b \left[\frac{\partial F}{\partial f}\eta(x) + \frac{\partial F}{\partial f'}\eta'(x)\right] dx = 0$$

Just as in Section 7.1, we treat the second term using integration by parts, so

$$\int_a^b \frac{\partial F}{\partial f'}\eta'(x)dx = \left[\frac{\partial F}{\partial f'}\eta(x)\right]_a^b - \int_a^b \frac{d}{dx}\left(\frac{\partial F}{\partial f'}\right)\eta(x)dx$$

The first term is zero because $\eta(a) = 0 = \eta(b)$, so our minimization condition becomes

$$\int_a^b \left[\frac{\partial F}{\partial f} - \frac{d}{dx}\frac{\partial F}{\partial f'}\right]\eta(x)\, dx = 0$$

Once again, since $\eta(x)$ is arbitrary, we can only satisfy this if the expression that multiplies $\eta(x)$, in square brackets, also zero. That is

$$\frac{\partial F}{\partial f} - \frac{d}{dx}\frac{\partial F}{\partial f'} = 0 \tag{7.4}$$

This is called the *Euler-Lagrange Equation*. Given $F[f(x), f'(x), x]$, it is a second order differential that we solve to find the function $f(x)$ that minimizes $S[f(x)]$.

Let's try it out for the straight line in Section 7.1. In that case

$$F[f(x), f'(x), x] = \sqrt{1 + (f'(x))^2} \tag{7.5}$$

Carrying out the calculations in (7.4) one by one, we have

$$\begin{aligned}
\frac{\partial F}{\partial f} &= 0 \\
\frac{\partial F}{\partial f'} &= \frac{f'(x)}{\sqrt{1 + (f'(x))^2}} \\
\frac{d}{dx}\frac{\partial F}{\partial f'} &= \frac{f''(x)}{\sqrt{1 + (f'(x))^2}} - \frac{[f'(x)]^2 f''(x)}{\left[1 + (f'(x))^2\right]^{3/2}}
\end{aligned}$$

Therefore, (7.4) becomes

$$\begin{aligned}
-\frac{f''(x)}{\left[1 + (f'(x))^2\right]^{1/2}} + \frac{(f'(x))^2 f''(x)}{\left[1 + (f'(x))^2\right]^{3/2}} &= -\frac{f''(x)}{\left[1 + (f'(x))^2\right]^{3/2}} \left[1 + (f'(x))^2 - (f'(x))^2\right] \\
&= -\frac{f''(x)}{\left[1 + (f'(x))^2\right]^{3/2}} = 0
\end{aligned}$$

which implies that

$$f''(x) = 0$$

In other words, $f(x) = mx + c$ for some constants m and c, a straight line.

7.2.1 Important special cases

There are two cases to mention, in which the Euler Lagrange equations reduce to something that is often much simpler to solve than (7.4). Both cases are because (7.4) can be partially integrated, depending on the form of F.

One is the case when $F[f(x), f'(x), x] = F[f'(x), x]$, that is F does not depend explicitly on f. Notice that in Section 7.1 we ended up showing that $f'(x)$ was a constant via (7.3), implying a straight line, whereas above, we showed instead that $f''(x) = 0$. Of course, both are the same, but why did we end up at different places when it seemed like we used the same approach?

The reason is because the functional (7.5) for the distance between two points does not depend on $f(x)$, but only on its derivative. That is $\partial F/\partial f = 0$ so (7.4) implies that

$$\frac{d}{dx}\frac{\partial F}{\partial f'} = 0 \qquad \text{so} \qquad \frac{\partial F}{\partial f'} = \text{constant} \qquad \text{when} \qquad F[f(x), f'(x), x] = F[f'(x), x] \tag{7.6}$$

which is precisely the statement we concluded with in (7.3).

The second case is $F[f(x), f'(x), x] = F[f(x), f'(x)]$, that is F does not depend explicitly on x. To exploit this, we first multiply (7.6) by $f'(x)$ to get

$$f'\frac{\partial F}{\partial f} - f'\frac{d}{dx}\frac{\partial F}{\partial f'} = 0$$

Next we realize that

$$\frac{d}{dx}\left(f'\frac{\partial F}{\partial f'}\right) = f''\frac{\partial F}{\partial f'} + f'\frac{d}{dx}\frac{\partial F}{\partial f'}$$

Therefore, the Euler Lagrange equation (7.6) becomes

$$f'\frac{\partial F}{\partial f} + f''\frac{\partial F}{\partial f'} - \frac{d}{dx}\left(f'\frac{\partial F}{\partial f'}\right) = \frac{d}{dx}\left(F - f'\frac{\partial F}{\partial f'}\right) - \frac{\partial F}{\partial x} = 0$$

However, the statement that F does not depend explicitly on x means that $\partial F/\partial x = 0$. So,

$$F - f'\frac{\partial F}{\partial f'} = \text{constant} \qquad \text{when} \qquad F[f(x), f'(x), x] = F[f(x), f'(x)] \tag{7.7}$$

We saw (7.6) applied to the shortest distance between two points, and we will apply (7.7) in Section 7.3. In classical mechanics, you will learn that (7.6) has to do with "conserved quantities", and (7.7) will be used to prove the conservation of energy.

7.2.2 Variational notation

A common notation is used which makes it much easier to work with functionals like $S[f(x)]$. If we write $\delta f = \epsilon\eta(x)$, we can interpret δf as a "small change in $f(x)$" over the range of x that we care about. In that sense,

$$\delta S = S[f(x) + \delta f(x)] - S[f(x)] = 0$$

is equivalent to finding a function $f(x)$ which minimizes S. We say that $S[f(x)]$ is *stationary* when $f(x)$ minimizes the functional. In terms of the explicit form (7.1) we have

$$\delta S = \delta \int_a^b F\left[f(x), f'(x), x\right] dx = \int_a^b \left[\frac{\partial F}{\partial f}\delta f + \frac{\partial F}{\partial f'}\delta f'\right] dx = 0$$

This makes it simple to write down the derivation of (7.4), with the manipulation of the δ's looking just like manipulations of differentials. That is

$$\int_a^b \left[\frac{\partial F}{\partial f}\delta f + \frac{\partial F}{\partial f'}\delta f'\right] dx = \frac{\partial F}{\partial f'}\delta f\Big|_a^b + \int_a^b \left[\frac{\partial F}{\partial f} - \frac{d}{dx}\frac{\partial F}{\partial f'}\right]\delta f\, dx = 0 \tag{7.8}$$

and we once again make the argument that $\delta f(x)$ is arbitrary, albeit "small", so the expression in square brackets must be itself zero.

7.2.3 More than one dependent variable

It is straightforward to generalize (7.1) to the case of more than one dependent variable. For example, if we have two dependent variables $f(x)$ and $g(x)$, then

$$S[f(x), g(x)] = \int_a^b F\left[f(x), f'(x), g(x), g'(x), x\right] dx \tag{7.9}$$

and we let both of them vary by "small' functions $\delta f(x)$ and $\delta g(x)$. You get

$$\begin{aligned} \delta S &= \int_a^b \left[\frac{\partial F}{\partial f}\delta f + \frac{\partial F}{\partial f'}\delta f' + \frac{\partial F}{\partial g}\delta g + \frac{\partial F}{\partial g'}\delta g'\right] dx \\ &= \int_a^b \left\{\left[\frac{\partial F}{\partial f} - \frac{d}{dx}\frac{\partial F}{\partial f'}\right]\delta f + \left[\frac{\partial F}{\partial g} - \frac{d}{dx}\frac{\partial F}{\partial g'}\right]\delta g\right\} dx = 0 \end{aligned}$$

Allowing $f(x)$ and $g(x)$ to vary independently means that each of the expressions in square brackets must be zero. Therefore, there are two separate Euler-Lagrange equations, namely

$$\frac{\partial F}{\partial f} - \frac{d}{dx}\frac{\partial F}{\partial f'} = 0 \qquad \text{and} \qquad \frac{\partial F}{\partial g} - \frac{d}{dx}\frac{\partial F}{\partial g'} = 0$$

The generalization to more than two dependent variables is obvious.

7.3 Example: The Brachistochrone Problem

Let's use this formalism now to attack a practical problem. Imagine that you have a bead of mass m sliding down along a wire with no friction. The wire starts at a point (x_1, y_1) and ends at a point (x_2, y_2), and you want to know the shape of the wire that lets the bead from the start to the end in the least amount of time.

This is known as the *brachistochrone* problem, from the Greek for "shortest time", and the answer is far from obvious. See the left side of Figure 7.1. Your first thought might be to take the shortest path length, that is, the straight line. Or maybe, you want to fall directly down first, to pick up the greatest speed, then move over to the final point. Or maybe it's somewhere in between.

To set up the problem, see the right side of Figure 7.1. Let the bead start out at the origin, and end up at the point $(x, y) = (a, b)$. The path traveled will be $y = f(x)$, and is fixed at the two endpoints. We want to find the function $f(x)$ that minimizes the time to fall under gravity. This is a clear example of a problem to be solved with the calculus of variations.

Our axes are defined with y going down. That is the bead moves in the $+y$ direction. The time dt it takes for the particle to move a distance $d\ell = \sqrt{dx^2 + dy^2}$ is $d\ell/v$ where v is the particle's speed. Since the bead starts from rest at the origin, conservation of energy says

$$\frac{1}{2}mv^2 - mgy = 0 \qquad \text{so} \qquad v = \sqrt{2gy}$$

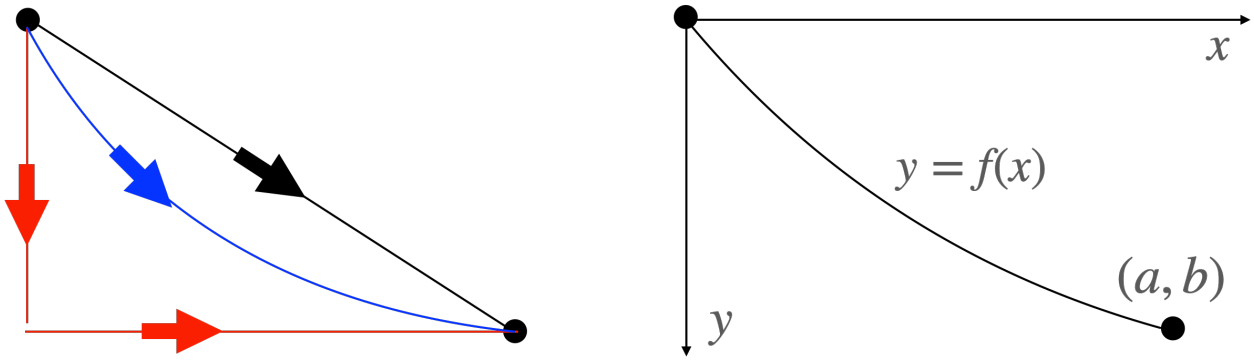


Figure 7.1: The brachistochrone problem is to find the path of shortest time for an object to fall between two points.The left diagram demonstrates that the answer is far from obvious. The right sets up the problem mathematically. Note that positive y is downward.

We can therefore write the time it takes for the bead to travel along the path $y = f(x)$ as

$$T[f(x)] = \int_{0,0}^{a,b} \frac{d\ell}{v} = \int_{0,0}^{a,b} \frac{\sqrt{dx^2 + dy^2}}{\sqrt{2gy}} = \frac{1}{\sqrt{2g}} \int_{0,0}^{a,b} \sqrt{\frac{1 + (f'(x))^2}{f(x)}}\, dx$$

Finding $f(x)$ that minimizes $T[f(x)]$ means to apply the Euler Lagrange equation (7.4) to

$$F[f(x), f'(x), x] = \sqrt{\frac{1 + (f'(x))^2}{f(x)}} = \left[\frac{1 + (f'(x))^2}{f(x)}\right]^{1/2}$$

This time $F[f(x), f'(x), x]$ does not explicitly depend on x, so we can use the Euler Lagrange equation as integrated in (7.7). That is

$$\begin{aligned} F - f' \frac{\partial F}{\partial f'} &= \left[\frac{1 + (f'(x))^2}{f(x)}\right]^{1/2} - \frac{1}{(f(x))^{1/2}} \frac{(f'(x))^2}{\left[1 + (f'(x))^2\right]^{1/2}} \\ &= \frac{1}{(f(x))^{1/2}} \frac{1}{\left[1 + (f'(x))^2\right]^{1/2}} = \text{constant} \equiv \frac{1}{c^{1/2}} \end{aligned}$$

Squaring both sides gives us the differential equation

$$f(x)\left[1 + (f'(x))^2\right] = c$$

where c is a constant that we will determine shortly from the boundary conditions.
If we write $y = f(x)$ the the differential equation becomes

$$\frac{dy}{dx} = \sqrt{\frac{c - y}{y}}$$

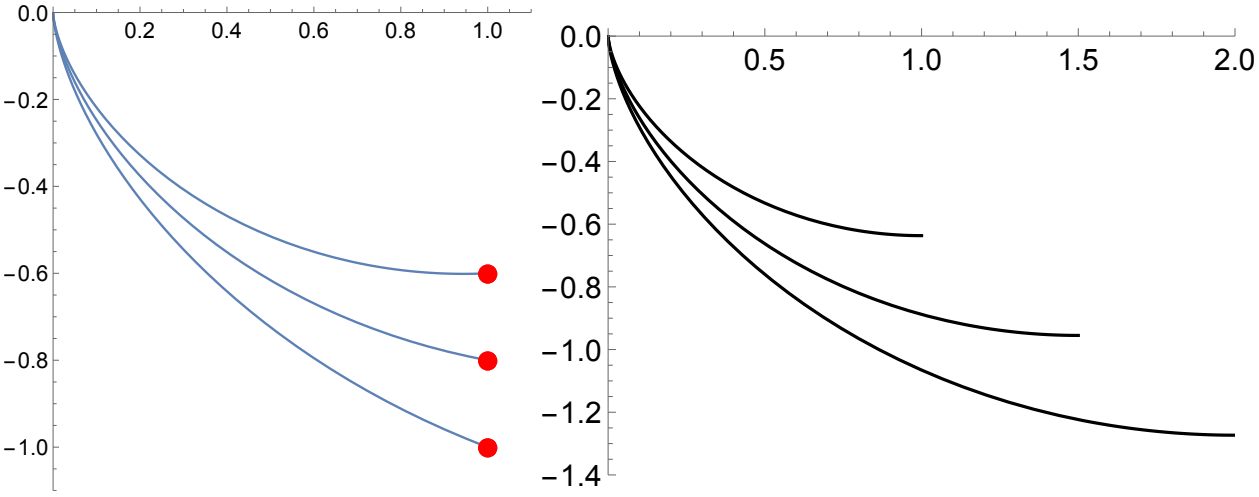


Figure 7.2: Different solutions to the brachistochrone problem. The left is where the endpoint is fixed. The right is when the vertical position of the endpoint is allowed to float.

where we note that, the way we have defined the axes in Figure 7.1, we expect the derivative to be positive. Writing this as

$$\sqrt{\frac{y}{c-y}}\,dy = dx$$

we see that the left side is easy to integrate if we make the substitution $y = c\sin^2\theta$. Then $c - y = c\cos^2\theta$ and $dy = 2c\sin\theta\cos\theta\,d\theta$, and

$$\frac{\sin\theta}{\cos\theta}\,2c\sin\theta\cos\theta\,d\theta = 2c\sin^2\theta\,d\theta = c(1-\cos 2\theta) = dx$$

Integrating this and putting it together with our substitution for y gives us

$$x = \frac{c}{2}(2\theta - \sin 2\theta) + d \tag{7.10a}$$

$$y = c\sin^2\theta \tag{7.10b}$$

where c and d are constants. These parametric equations describe a curve called a *cycloid*, which is usually described as the path of a point on the rim of a wheel of radius c. It apparently is also the shape of the path that minimizes the travel time between two points for a bead subject to gravity.

To complete the problem, we have to determine c and d. Since $\theta = 0$ gives $y = 0$ and $x = d$, it is clear that $d = 0$ since the curve includes the origin. Therefore (7.10) can then be solved for c and the value of θ that gives $(x, y) = (a, b)$. This typically requires a numerical solution, which is not hard to do in MATHEMATICA.

Figure 7.2 on the left shows the solution for the endpoints (a, b), each with $a = 1$ and $b = 0.6$, 0.8, and 1.0. (I did not bother to reverse the sign of the vertical axis.)

Interestingly, we can find solutions if we instead provide only the value of a, and let the vertical position of the endpoint float. This would seem to spoil our formalism, where we required that the endpoints be fixed. However, looking back at our derivation of the Euler Lagrange equations in (7.8), we could instead require that $\partial F/\partial f' = 0$ at the endpoint. In our case, this means that

$$\frac{1}{(f(x))^{1/2}} \frac{f'(x)}{\left[1 + (f'(x))^2\right]^{1/2}} = 0 \qquad \text{for} \qquad x = a$$

which in turn implies that the slope $y' = 0$ at $x = a$. From (7.10) this implies that

$$c \sin 2\theta = 0 \qquad \text{when} \qquad a = c\theta = c\pi/2$$

Plots with this approach, for $a = 1$, 1.5, and 2.0 are shown on the right in Figure 7.2.

7.4 Example with Constraints: Lagrange Multipliers

It is not uncommon to have a variational calculus problem that involves *constraints* on the quantities involved. There is a general approach to all such problems that involves the use of *Lagrange Multipliers*. We will illustrate the approach here with one type of constraint, namely a different integral over the same independent variable which has to be kept at a fixed value.

Once again, our problem is to find the function $f(x)$ which minimizes the functional

$$S = \int_a^b F\left[f(x), f'(x), x\right] dx \tag{7.11}$$

This time, however, there is a constraint that the quantity

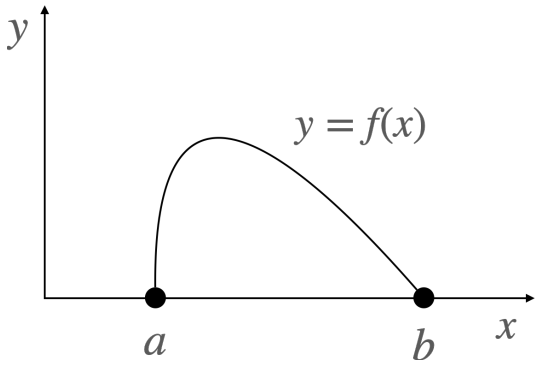
$$L = \int_a^b G\left[f(x), f'(x), x\right] dx \tag{7.12}$$

must be kept constant. For example, L might represent the length of the curve $y = f(x)$. Keeping L constant is the same as writing $\delta L = 0$ as we vary $\delta f(x)$. Since $\delta S = 0$ for the correct $f(x)$, we can get a modified form of the Euler-Lagrange equation by writing

$$\delta(S + \lambda L) = \delta \int_a^b \left\{F\left[f(x), f'(x), x\right] + \lambda G\left[f(x), f'(x), x\right]\right\} dx = 0 \tag{7.13}$$

for some constant λ. This modified Euler-Lagrange equation will automatically include the constraint (7.12). An additional constant λ, known as Lagrange multiplier, will be included in the differential equation for $f(x)$ that results, but it can be determined using the constraint equation.

Figure 7.3: An example of a calculus of variations problem with an integral constraint. The goal is to find the function $y = f(x)$ which is fixed to the x-axis at $x = a$ and $x = b$ and which encloses the maximum area underneath it, subject to the constraint that the length $L > b-a$ of the curve is fixed. You can think of the curve as a fixed length of rope.



You will see this in an advanced course in classical mechanics, where the Lagrange multipliers turn out to be the "forces" which lead to constrained motion of a system. See, for example, Section 19 of "Theoretical Mechanics of Particles and Continua" by Fetter and Walecka.

Let's again illustrate this approach with a specific problem. Figure 7.3 A "rope" of fixed length L is attached to the x-axis between the points $x = a$ and $x = b$. The job is to find the shape of the rope which maximizes the area it encloses over the x-axis. We are therefore looking to maximize the functional

$$S[f(x)] = \int_a^b f(x)\,dx$$

subject to the constraint that

$$L = \int_a^b ds = \int_a^b \left[1 + (f'(x))^2\right]^{1/2} dx$$

remains fixed. The modified Euler-Lagrange equation is derived from

$$\begin{aligned}
\delta(S + \lambda L) &= \delta \int_a^b \left\{ f(x) + \lambda \left[1 + (f'(x))^2\right]^{1/2} \right\} dx \\
&= \int_a^b \left\{ \delta f(x) + \lambda \frac{f'(x)}{\left[1 + (f'(x))^2\right]^{1/2}} \delta f'(x) \right\} dx \\
&= \lambda \frac{f'(x)}{\left[1 + (f'(x))^2\right]^{1/2}} \delta f(x) \Bigg|_a^b + \int_a^b \left\{ 1 - \lambda \frac{d}{dx} \frac{f'(x)}{\left[1 + (f'(x))^2\right]^{1/2}} \right\} \delta f(x)\,dx = 0
\end{aligned}$$

where we once again make use of integration by parts. Now, as we have observed previously, the first term on the right hand size is zero because $\delta f(a) = \delta f(b) = 0$. That is, the endpoints of the rope are fixed to the x-axis. Also as before, $\delta f(x)$ is arbitrary, so to have the integral equal to zero implies that

$$1 - \lambda \frac{d}{dx} \frac{f'(x)}{\left[1 + (f'(x))^2\right]^{1/2}} = 0$$

This is the differential equation we need to solve in order to come up with the function $y = f(x)$. This form is easy to integrate once, and we get

$$\frac{\lambda f'(x)}{\left[1 + (f'(x))^2\right]^{1/2}} = x + c$$

for some constant c. Squaring both sides and writing $dy/dx = f'(x)$ we get the differential equation

$$\lambda^2 \left(\frac{dy}{dx}\right)^2 = (x+c)^2 \left[1 + \left(\frac{dy}{dx}\right)^2\right] \qquad \text{so} \qquad dy = \frac{x+c}{[\lambda^2 - (x+c)^2]^{1/2}}\, dx$$

The right side is not hard to integrate if we make the substitution

$$x + c = \lambda \sin t \qquad \text{so} \qquad dx = \lambda \cos\theta\, d\theta$$

in which case the differential equation becomes

$$dy = \frac{\lambda \sin\theta}{\lambda \cos\theta}\, \lambda \cos\theta\, d\theta = \lambda \sin\theta\, d\theta \qquad \text{so} \qquad y + c' = -\lambda \cos\theta$$

where c' is some other constant. It is simple to eliminate the variable θ, and we get

$$(x+c)^2 + (y+c')^2 = \lambda^2$$

The answer is a circular arc, probably what you would have guessed. The Lagrange multiplier λ has an obvious physical interpretation as the radius of the circle. In order to find c and c', we need to solve

$$\begin{aligned} (a+c)^2 + (c')^2 &= \lambda^2 \\ \text{and} \qquad (b+c)^2 + (c')^2 &= \lambda^2 \end{aligned}$$

for c and c', in terms of a, b, and λ. Subtracting these two equations gives $a + c = \pm(b + c)$, but the plus sign gives nonsense, so $c = (a + b)/2$. The result is simpler if we translate the x-axis so that $a = -x_0$ and $b = x_0$ which means that $c = 0$ and $c' = \pm(\lambda^2 - x_0^2)^{1/2}$. Clearly, as you would have expected, the radius λ of the circle has to be at least as large as the displacement of the fixed points from the origin.

We see that the center of the circle is along the y axis, at a distance c' above (or below) the x-axis. If θ represents the angular variable that traces the circle, then $\tan\theta = \pm x_0/c'$ gives the range of angles $\Delta\theta = 2\tan^{-1}(x_0/c')$ that are excluded from the circle. The length constraint then becomes

$$L = (2\pi - \Delta\theta)\lambda$$

However, it is more important to realize the physical interpretation of λ, namely the radius of the circle. Sure, if we want to fully solve the problem to find the shape of the curve that

maximizes the area for these fixed points and length, this is what we need. However, the "physics" is more in the interpretation, and that's usually what's really important.

There's one other question, which in fact bothers me because I don't know how to answer it. We wrote our functional as "the area under a curve $y = f(x)$" which apparently implies that $f(x)$ is a single valued function that sits above the x-axis. However, we've come up with a solution that isn't (necessarily) single valued if the rope is long enough, and that can also be below the axis. Perhaps understanding "below the axis" isn't so hard - it's the minimum, not the maximum - and maybe the fact that we were careless with signs when squaring things and taking square roots explains the lack of single-valuedness. Nevertheless, I thought I would mention it.

Chapter 8

Functions of a Complex Variable

We have been rather cavalier about complex variables throughout this book so far. After mentioning them only briefly in Section 1.1.1, we made use of them from time to time when it was handy. Probably most useful was the relationship

$$z = x + iy = re^{i\phi} = r\cos\phi + i\,r\sin\phi$$

which showed how to represent a complex number z in terms of two real numbers x and y which identified a point in the complex plane with Cartesian coordinates, or in terms of two different real numbers r and ϕ which identify the same point but in plane polar coordinates. The connection was made using Euler's Formula, which we "derived" in Section 2.4.

This chapter will get much more serious about complex variables, in particular by discussing the theory and applications of *functions* of complex variables. These functions are mappings $\mathbb{C} \mapsto \mathbb{C}$, which we can write generically as

$$w = f(z) = u(x,y) + iv(x,y) \qquad \text{where} \qquad z = x + iy \tag{8.1}$$

with $x, y, u, v \in \mathbb{R}$ and $z, w \in \mathbb{C}$. In fact, it will be useful to realize that these functions are also mappings $\mathbb{R}^2 \mapsto \mathbb{R}^2$, which means they should have properties of functions in two spacial dimensions. Indeed, we'll borrow some things we proved about vector calculus in Chapter 4.

8.1 Differentiability and Convergence

It can seem that the generalization to complex functions from real functions is simple, and not worth a lot of discussion, but in fact that is not the case. I will illustrate this with a couple of examples of fundamental differences between real and complex functions.

First our first example, consider the real function

$$f(x) = 2\int_0^x |x'|\,dx' = \begin{cases} +x^2 & x \geq 0 \\ -x^2 & x \leq 0 \end{cases} \tag{8.2}$$

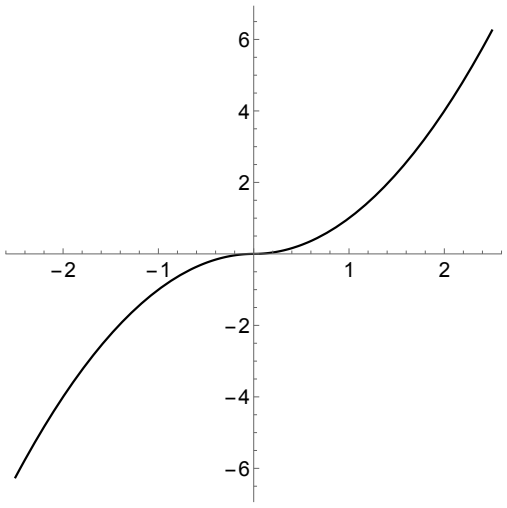


Figure 8.1: A plot of the (real) function given by (8.2). This is a smooth, that is continuous, function, passing through the point $(x, y) = (0, 0)$. It also has a well defined derivative, equal to zero, at $x = 0$. However, higher derivatives do not exist at $x = 0$. We will see that you can never have this situation with a complex function. That is, if it is differentiable once, then it it is differentiable an infinite number of times.

which is plotted in Figure 8.1. It looks like a perfectly reasonable continuous function passing through the origin. In fact, it has a perfectly definable derivative as $x = 0$. That is, taking ϵ to be positive,

$$f'(x) = \lim_{\epsilon\to 0} \frac{f(+\epsilon) - f(-\epsilon)}{2\epsilon} = \lim_{\epsilon\to 0} \frac{(+\epsilon)^2 - (-(-\epsilon)^2)}{2\epsilon} = \lim_{\epsilon\to 0} \frac{2\epsilon^2}{2\epsilon} = \lim_{\epsilon\to 0} \epsilon = 0$$

What's more, the first derivative is continuous at $x = 0$, since $f(x) = 2x$ for $x > 0$ and $f(x) = -2x$ when $x < 0$, and both of these approach $f'(0)$ for $x \to 0$, regardless of whether I approach from the negative of positive direction.

However, there is a problem with the second derivative. For $x > 0$, it is clear that $f''(x) = +2$, but for $x < 0$, $f''(x) = -2$. There is a clear discontinuity in the second derivative at $x = 0$. That is, $f''(0)$ does not exist, even though the function and its first derivative both exist and are continuous.

We will learn that this never happens for functions of a complex variable. If a function is differentiable once, then it will be differentiable an infinite number of times. This is due to the property of *analyticity*, which we will cover in Section 8.3. The catch is that in order for a complex function to be analytic, it needs to satisfy a particularly stringent condition.

Now a second example. Consider the (real) function

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

This is perfectly well defined for all real numbers. However, if we perform a Taylor expansion about $x = 0$ we find

$$f(x) = 1 - x^2 + x^4 - x^6 + \cdots$$

and we are going to get into trouble for $|x| \geq 1$. We might have expected something like this if the function were $1/(1 - x^2)$ because it would be ill defined at $x = \pm 1$. The problem

here is that if we made the function complex, that is

$$f(z) = \frac{1}{1+z^2}$$

then it would be ill defined for $z = \pm i$. We therefore say that this function, as well as the function $1/(1-x^2)$, have *radii of convergence* given by $|z| < 1$. Obviously, the idea of functions of real numbers is somehow incomplete, and we need to consider what happens when we extend the function into the complex plane.

We will see that it becomes natural to think of functions of real variables as a special case of functions of complex variables. In fact, we will find that doing things like integrating real functions is better thought of in terms of integrals over some path in the complex plane.

First, though, let's do some preliminary and simple investigations of the properties of complex functions.

8.2 Examples of Complex Functions

In this section we will go through various specific examples of complex functions written in the form (8.1). We'll refer back to these examples when we study more fundamental properties of analytic functions.

8.2.1 Power laws

First consider $w = f(z) = z^2$ where $z = x + iy$. It is simple to put this in the form (8.1). We naturally write

$$w = z^2 = (x+iy)^2 = x^2 - y^2 + 2ixy = u(x,y) + iv(x,y) \tag{8.3a}$$

where

$$u(x,y) = x^2 - y^2 \qquad \text{and} \qquad v(x,y) = 2xy \tag{8.3b}$$

We can think about the derivative of $w = f(z)$ with respect to z. We sort of expect the answer to be $f'(z) = 2z$, but can we prove it? We would proceed to write

$$f'(z) = \frac{dw}{dz} = \lim_{\Delta z \to 0} \frac{f(z+\Delta z) - f(z)}{\Delta z} = \lim_{\Delta z \to 0} \frac{(z+\Delta z)^2 - z^2}{\Delta z} = \lim_{\Delta z \to 0} \frac{2z\Delta z + (\Delta z)^2}{\Delta z}$$

but we have to be aware of a potential complication, because $\Delta z = \Delta x + i\Delta y$, so Δz can approach zero in various ways, depending on how you take the limits $\Delta x \to 0$ and $\Delta y \to 0$. Writing this all out, and tossing out higher orders in Δx and Δy, we find

$$f'(z) = \lim_{\Delta x \to 0, \Delta y \to 0} \frac{2(x+iy)(\Delta x + i\Delta y)}{\Delta x + i\Delta y}$$

and now you can see clearly that if we take $\Delta z \to 0$ by, first, putting $\Delta y = 0$ and then taking $\Delta x \to 0$, or, second, putting $\Delta x = 0$ and then taking $\Delta y \to 0$, then in either case we get $f'(z) = 2(x + iy) = 2z$.

In fact, we can be more general and write $\Delta y = a\Delta x$ for some constant a, in which case

$$f'(z) = \lim_{\Delta x \to 0} \frac{2(x + iy)\Delta x(1 + ia)}{\Delta x(1 + ia)} = 2(x + iy) = 2z$$

so we are confident that the derivative is what we expect. We will investigate the general circumstances under which the derivative of a complex function makes sense in Section 8.3.

It follows directly from this analysis that higher powers of positive integers are also well defined and differentiable. This means that infinite series of the form

$$f(z) = \sum_{n=0}^{\infty} c_n z^n$$

are also well defined.

Powers that are not positive integers, however, can be problematic. For example, functions that include terms or factors like

$$f(z) = \frac{1}{z} \qquad \text{or} \qquad f(z) = \frac{1}{z - z_0}$$

are of course singular at $z = 0$ or $z = z_0$, so are not differentiable there. We say that these functions of *poles* at $z = 0$ or $z = z_0$.

Different difficulties arise for non-integer positive powers. For example, consider the function

$$f(z) = z^{1/2}$$

It is easiest to analyze this by expressing z in polar coordinates, that is $z = re^{i\phi}$, so

$$f(z) = r^{1/2} e^{i\phi/2}$$

Now if $\phi \to \phi + 2\pi$, then $z \to re^{i(\phi+2\pi)} = re^{i\phi}e^{2\pi i} = re^{i\phi}$ so z is unchanged. However

$$f(z) \to r^{1/2} e^{i(\phi+2\pi)/2} = r^{1/2} e^{i\phi/2} e^{i\pi} = -r^{1/2} e^{i\phi/2}$$

That is, $f(z)$ changes sign. Therefore, we need to agree on a "standard" range of the phase ϕ, and that is $-\pi/2 < \phi \leq +\pi/2$.

8.2.2 Special functions

Most of the special functions discussed in Sections 1.5 and 3.6 are more generally expressed as functions of a complex variable $z = x + iy$. It is easiest to start with

$$f(z) = e^z = e^x e^{iy}$$

from which we can define

$$\cos z = \frac{e^{iz} + e^{-iz}}{2} \qquad \text{and} \qquad \sin z = \frac{e^{iz} - e^{-iz}}{2i}$$
$$\text{and} \qquad \cosh z = \frac{e^{z} + e^{-z}}{2} \qquad \text{and} \qquad \sinh z = \frac{e^{z} - e^{-z}}{2}$$

For the logarithm, we naturally write $z = re^{i\phi}$ and so

$$\log z = \log r + i\phi$$

where now it is obvious that we need to stick to the standard range of ϕ.

8.2.3 Peculiar examples

We can also define some oddball functions like

$$f(z) = z^* = x - iy \qquad \text{and} \qquad f(z) = |z| = (x^2 + y^2)^{1/2}$$

Taking derivatives of these sorts of things will turn out to be problematic.

8.3 Analyticity

If a function of a complex variable has a derivative that exists at some point in the complex plane, then we say that the function is analytic at that point. We saw in Section 8.2.1 that we needed to consider approaching from either the x or y direction, or any direction for that matter, when calculating the derivative of the function $f(z) = z^2$. In this section we will formalize this requirement for general functions of a complex variable.

8.3.1 Cauchy-Riemann relations

Go back to the basics and you'll see a potential problem. If you approach the limit to the point (x, y) in the complex plane along a line of constant y, then

$$\begin{aligned} \frac{dw}{dz} &= \lim_{\epsilon\to 0} \frac{f(z+\epsilon) - f(z)}{\epsilon} \\ &= \lim_{\epsilon\to 0} \frac{u(x+\epsilon, y) - u(x,y)}{\epsilon} + i \lim_{\epsilon\to 0} \frac{v(x+\epsilon, y) - v(x,y)}{\epsilon} \\ &= \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x} \end{aligned} \tag{8.4}$$

On the other hand, if you approach along a line of constant x, then

$$\begin{aligned}\frac{dw}{dz} &= \lim_{\epsilon\to 0}\frac{f(z+i\epsilon)-f(z)}{i\epsilon} \\ &= \frac{1}{i}\lim_{\epsilon\to 0}\frac{u(x,y+\epsilon)-u(x,y)}{\epsilon}+\lim_{\epsilon\to 0}\frac{v(x,y+\epsilon)-v(x,y)}{\epsilon} \\ &= -i\frac{\partial u}{\partial y}+\frac{\partial v}{\partial y} \end{aligned} \tag{8.5}$$

Therefore, in order to consistently define the derivative, we must have

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \tag{8.6a}$$

$$\text{and} \qquad \frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y} \tag{8.6b}$$

These are called the *Cauchy-Riemann Relations*. Any function $f(z)$ which obeys these relations is called *analytic*.

Now just because we've come up with conditions based on ϵ approaching zero along lines of constant x or constant y, doesn't mean that the derivative works for $\epsilon \to 0$ from any direction. It may seem reasonable because we showed it works for two orthogonal directions, but there are more restrictions that that. I won't go into these details, but for our purposes, we can just assume that a function $f(z)$ is analytic if and only if (8.6) hold.

Let's do a couple of examples, starting with $f(z) = z^2$. See (8.3). We have

$$\frac{\partial u}{\partial x} = \frac{\partial}{\partial x}(x^2-y^2) = 2x \qquad \text{and} \qquad \frac{\partial v}{\partial y} = \frac{\partial}{\partial y}(2xy) = 2x$$

so (8.6a) is satisfied. We also have

$$\frac{\partial v}{\partial x} = \frac{\partial}{\partial x}(2xy) = 2y \qquad \text{and} \qquad \frac{\partial u}{\partial y} = \frac{\partial}{\partial y}(x^2-y^2) = -2y$$

and (8.6b) is also satisfied. Therefore, the function is analytic. In fact, it is analytic for every z in the complex plane. We therefore say that the function is *entire*.

Now consider $f(z) = z^*$ so that $u(x,y) = x$ and $v(x,y) = -y$. This satisfies (8.6b), but violates (8.6a), i.e. "$1 = -1$", everywhere. This function is analytic nowhere in the complex plane.

It is easy to see that if $f(z)$ is analytic at a point z, then $f'(z)$ is also analytic at z. In other words, if $f(z)$ is differentiable once at z, then it is differentiable an infinite number of times. If we write (8.6) as

$$\frac{\partial u}{\partial x}-\frac{\partial v}{\partial y} = 0 \qquad \text{and} \qquad \frac{\partial v}{\partial x}+\frac{\partial u}{\partial y} = 0$$

and the derivative of $f(z)$ as

$$f'(z) = \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x} = \frac{\partial v}{\partial y} - i\frac{\partial u}{\partial y}$$

then to check for analyticity, we write

$$\frac{\partial}{\partial x}\frac{\partial u}{\partial x} - \frac{\partial}{\partial y}\frac{\partial v}{\partial x} = \frac{\partial}{\partial x}\frac{\partial v}{\partial y} - \frac{\partial}{\partial y}\frac{\partial v}{\partial x} = 0$$

assuming that $u(x, y)$ and $v(x, y)$ are well enough behaved so that we can switch the order or of differentiation. Therefore (8.6a) is satisfied for $f'(z)$. We also check

$$\frac{\partial}{\partial x}\left(-\frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial y}\frac{\partial v}{\partial y} = -\frac{\partial}{\partial x}\frac{\partial u}{\partial y} + \frac{\partial}{\partial y}\frac{\partial u}{\partial x} = 0$$

and (8.6b) is satisfied. Therefore, the derivative is also analytic.

8.4 Contour Integration

It should be clear that if we are going to integrate some function $f(z)$ between z_1 and z_2, then we'll need to specify the path we take in the complex plane to connect these two complex numbers. Consequently, complex integration, generally referred to as *contour integration*, will make use of many of the techniques we developed in Chapter 4, especially Section 4.3.

It is not too hard to turn a contour integral into a set of real integrals. If C is the curve along we wish to integrate from $z_1 = x_1 + iy_1$ to $z_2 = x_2 + iy_2$, then

$$\begin{aligned}
\int_C f(z)\,dz &= \int_C [u(x,y) + iv(x,y)]\,[dx + i\,dy] \\
&= \int_C [u(x,y)\,dx - v(x,y)\,dy] + i\int_C [v(x,y)\,dx + u(x,y)\,dy] \qquad (8.7) \\
&= \int_{t_1}^{t_2} \left[u(x,y)\frac{dx}{dt} - v(x,y)\frac{dy}{dt}\right] dt + i\int_{t_1}^{t_2} \left[v(x,y)\frac{dx}{dt} + u(x,y)\frac{dy}{dt}\right] dt \qquad (8.8)
\end{aligned}$$

where the form (8.8) makes use of an assumed parameterization of the curve by the functions $x(t)$ and $y(t)$. This in fact would be a practical way to carry out the integral.

For example, suppose we want to integrate from $(x_1, y_1) = (1, 0)$ to $(x_2, y_2) = (-1, 0)$ along a semicircle C traced counter clockwise through the upper half of the complex plane. Then $x(t) = \cos t$, $y(t) = \sin t$, $t_1 = 0$, and $t_2 = \pi$. For the function $f(z) = z = x + iy$, we have

$$\begin{aligned}
\int_C f(z)\,dz &= \int_0^\pi [\cos t(-\sin t) - \sin t(\cos t)]\,dt + i\int_0^\pi [\sin t(-\sin t) + \cos t(\cos t)]\,dt \\
&= \int_0^\pi 2\sin t\cos t\,dt + i\int_0^\pi \left[\cos^2 t - \sin^2 t\right]\,dt = \int_0^\pi \sin 2t\,dt + i\int_0^\pi \cos 2t\,dt \\
&= -\frac{1}{2}\cos 2t\Big|_0^\pi + i\,\frac{1}{2}\sin 2t\Big|_0^\pi = 0
\end{aligned}$$

This might seem like a peculiar result, but there are a number of peculiar results when doing contour integration of complex functions. Some of these peculiar results are very useful for solving problems in Physics.

Now consider the integral along the same contour but for the function

$$f(z) = \frac{1}{z} = \frac{1}{z}\frac{z^*}{z^*} = \frac{x - iy}{x^2 + y^2}$$

The denominator $x^2 + y^2 = 1$ along this contour, and $u = x$ and $v = -y$, so

$$\begin{aligned}\int_C f(z)\,dz &= \int_0^\pi [\cos t(-\sin t) + \sin t(\cos t)]\,dt + i\int_0^\pi [-\sin t(-\sin t) + \cos t(\cos t)]\,dt \\ &= 0 + i\int_0^\pi \left[\cos^2 t + \sin^2 t\right]\,dt = i\int_0^\pi dt = \pi i\end{aligned}$$

and the result is once again peculiar.

Note that the contour we follow makes an important difference. In the second example above, if we went from $(x_1, y_1) = (1, 0)$ to $(x_2, y_2) = (-1, 0)$ but along a semicircle C traced clockwise through the lower half of the complex plane, we would have found the integral to be $-\pi i$ instead of $+\pi i$.

8.4.1 Integral around a closed loop

It is pretty easy to see that if our contour in the two examples of the previous section was a closed loop, starting and ending at $(x, y) = (1, 0)$, along a circular contour C traced counter clockwise, then we would have found

$$\oint_C z\,dz = 0 \qquad \text{and} \qquad \oint_C \frac{1}{z}\,dz = 2\pi i$$

This is actually a hint of two very useful theorems that we will now discuss.

First, rewrite (8.7) in terms of two real line integrals in the (x, y) plane using $\vec{A} \equiv u\hat{i} - v\hat{j}$ and $\vec{B} \equiv v\hat{i} + u\hat{j}$ as

$$\oint_C f(z)\,dz = \oint_C \vec{A}\cdot d\vec{r} + i\oint_C \vec{B}\cdot d\vec{r}$$

If C is a closed contour, then we can write each of these two integrals using Stoke's Theorem (Section 4.3.1). Applying the Cauchy-Riemann relations (8.6), we find

$$\oint_C \vec{A}\cdot d\vec{r} = \left[\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right]\hat{k} = 0 \qquad \text{and} \qquad \oint_C \vec{B}\cdot d\vec{r} = \left[\frac{\partial v}{\partial y} - \frac{\partial u}{\partial x}\right]\hat{k} = 0$$

This proves the *Cauchy-Goursat Theorem*, namely that the integral around any closed contour of any function that is analytic throughout the enclosed region is zero. This explains the result for the example above when $f(z) = z$. We did the integral over a circular contour,

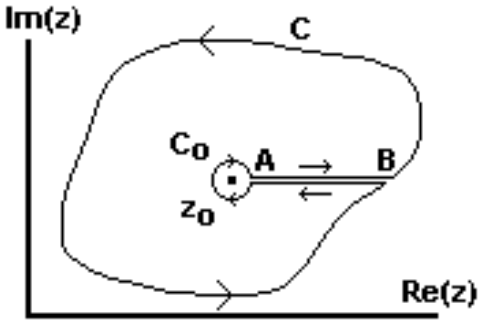


Figure 8.2: A closed contour C in the complex plane which has a section C_0, traversed in the "wrong" direction, that avoids the pole at $z = z_0$. An integral around C_0 in the "right" (that is, counter clockwise) direction can be added to the integral around C to get an integral around C that includes the pole, because the integral around C, as shown, is zero.

but, in fact, it didn't matter whether the contour was circular or not, only that it was closed, since $f(z) = z$ is analytic everywhere.

Note that a corollary of the Cauchy-Goursat Theorem is that the contour integral of an analytic function $f(z)$ between z_1 and z_2 is independent of the contour. This is easy to see. If one of the contours from z_1 to z_2 is reversed, so goes from z_2 to z_1, then the integral picks up a minus sign. We now have a closed contour, though, that is $z_1 \to z_2 \to z_1$, so the sum of the two integrals must be zero. That is, the two integrals $z_1 \to z_2$ must equal each other.

Of course, the reason we don't get zero when $f(z) = 1/z$ is that this function is not analytic at $z = 0$. In this case, however, there is the *Cauchy Integral Theorem* which states that

$$\oint_C \frac{f(z)}{z - z_0}\, dz = 2\pi i f(z_0) \tag{8.9}$$

where C is a closed contour containing the point $z = z_0$ and $f(z)$ is analytic inside C. As usual, we assume the contour is traced in a counter clockwise direction.

It is not hard to prove (8.9). In fact, we've already done most of the work. We can replace any arbitrary contour C that encloses $z = z_0$ with a small circular contour C_0 about the pole, plus the contour shown in Figure 8.2. The integrals along $A \to B$ and $B \to A$ cancel each other out, so we can replace the integral around C with the integral around C_0. Since the radius of C_0 is arbitrarily small, we can take $f(z_0)$ out of the integral, leaving us with the integral of $1/(z - z_0)$, which we have already shown to be equal to $2\pi i$, after translating the axis to put z_0 at the origin. If you want to be more formal about it, write $z - z_0 = re^{i\theta}$ and integrate over $0 \le \theta \le 2\pi$ with $dz = ire^{i\theta}\, d\theta$. This proves (8.9).

8.4.2 Practical mathematical examples

The Cauchy Integral Theorem (8.9) makes it possible to do many definite integrals which might otherwise seem to be intractable. It is best to illustrate this with a specific example, although different examples might use different, but similar, approaches.

Consider the integral

$$\mathcal{I} = \int_0^\infty \frac{\cos x}{1 + x^2}\, dx \tag{8.10}$$

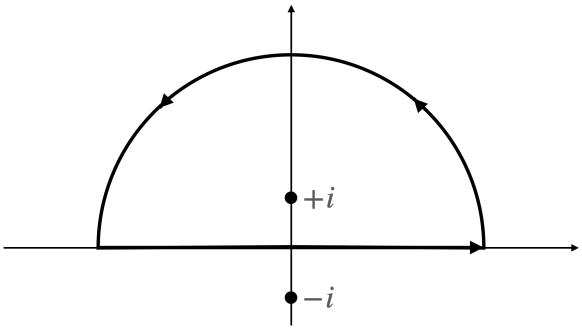


Figure 8.3: A contour in the complex plane used to evaluate the integral (8.10). The contour is traced counter clockwise, and the radius of the semicircle is taken to infinity. The integrand goes to zero along the semicircle, leaving only the contribution from the x-axis. However, the integral is actually evaluated using (8.9) and the pole at $z_0 = +i$.

which in fact can be written as a contour integral of the form (8.9) in which case it is simple to read off the answer. First, realize that the integrand is an even function, and that if I replace the cosine with a sine function, it would be an odd function. This means that

$$\mathcal{I} = \frac{1}{2}\int_{-\infty}^{\infty} \frac{\cos x}{1+x^2}\,dx = \frac{1}{2}\int_{-\infty}^{\infty} \frac{\cos x}{1+x^2}\,dx + i\frac{1}{2}\int_{-\infty}^{\infty} \frac{\sin x}{1+x^2}\,dx = \frac{1}{2}\int_{-\infty}^{\infty} \frac{e^{ix}}{1+x^2}\,dx$$

The final form can be equated to a contour integral, using the contour shown in Figure 8.3. The contour C runs along the x-axis in the positive direction, for some finite length symmetric with the y-axis, and closes with a semicircle in the *upper* hemisphere, returning to the x-axis. We choose the upper hemisphere because we want the integrand to go to zero as the radius of the semicircle goes to infinity. The denominator of the integrand tends to infinity for either the upper or lower hemisphere, but the numerator only goes to zero in the upper hemisphere. This is because the imaginary part of z is large and positive, so the exponential e^{ix} becomes small.

Furthermore, as the radius of C goes to infinity, the contour includes the entire real axis. In other words, for the contour C in Figure 8.3,

$$\mathcal{I} = \frac{1}{2}\oint_C \frac{e^{iz}}{1+z^2}\,dz$$

which is straightforward to evaluate using (8.9). We have

$$\mathcal{I} = \frac{1}{2}\oint_C \frac{e^{iz}}{(z+i)(z-i)}\,dz = 2\pi i\frac{1}{2}\left.\frac{e^{iz}}{z+i}\right|_{z=+i} = \frac{\pi}{2e}$$

which is verified in MATHEMATICA with Integrate[Cos[x]/(1 + x^2), {x, 0, ∞}].

Chapter 9

Probability and Statistics

The notions of probability and probability distributions are central to many fields of physics. Most notable of these are statistical thermodynamics and quantum mechanics, not to mention experimental physics in general. This chapter will lay down some of the basic mathematics associated with these areas.

If there are a number n of potential different outcomes from some experiment or measurement, and all of these different outcomes are equally probable, then coming up with any one of them has a probability of just $1/n$. If the outcomes are not equally probable, then we speak of a *probability distribution* of any one of those outcomes. This distribution is some function of the different outcomes, labeled in whichever way is appropriate. If I sum this function over the different possible outcomes (or integrate it if the outcomes are continuous) then you have to get unity.

When you do an experiment, in which the outcomes of some measurement can be sorted numerically, a natural way to present the data is using a *histogram*. Unless the amount of data is very large, the histogram will be an approximation to the *shape* of the distribution, because there will be some statistical fluctuations in each of the groups of measurements.

We are going to start this chapter by "throwing dice." This is a good way to illustrate all of these concepts. After that, we'll get more formal with the mathematics, and then extend these concepts.

9.1 Throwing Dice

Dice are a prototype for learning about probability and probability distributions. Dice are little cubes – the singular is "die" – with each side labeled with one through six dots. See Figure 9.1. If you throw any one die (and it is "fair") then there is an equal probability of getting any of the faces to land up. That is, the probability of getting a "one" is 1/6, the same as the probability of getting a "five", and so on.

Now imagine that you throw a handful of six dice at the same time, count the number of

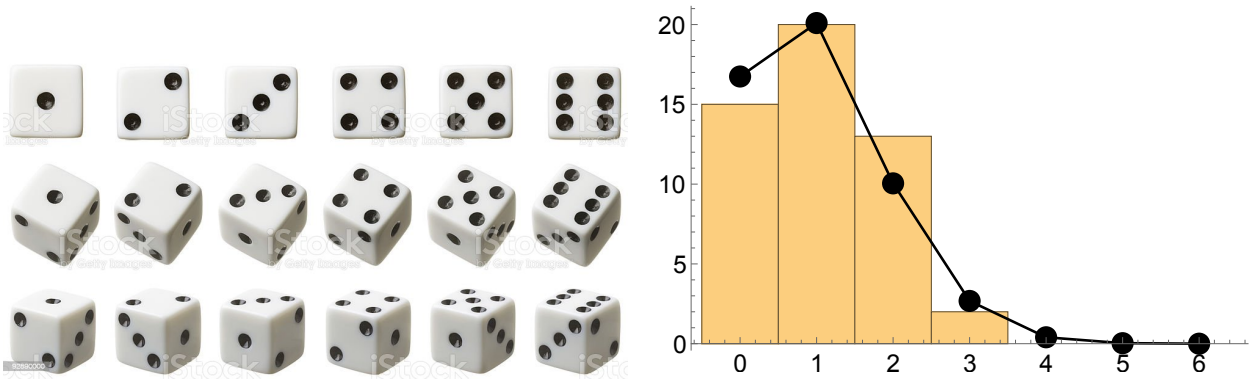


Figure 9.1: Six dice, viewed from different angles, showing each of the six faces. The right shows the result of an experiment, compared to the expected (average) result, of throwing a handful of six dice and counting the number of them that land with a "one" face up.

dice that land with a "one" face up, and then repeat the experiment several or many more times. The result of each throw will be a number between zero and six. It seems likely that one or two of the dice might land with a "one" face up, but it seems very unlikely that, for example, all six will land this way. Our goal is to try to understand these probabilities mathematically.

Figure 9.1 also shows the result of such an experiment, throwing fifty handfuls of six dice and each time counting the number that land with a "one" facing up. (Actually, I did not throw fifty handfuls of dice, but instead generated the data using the random number facility in MATHEMATICA.) The result of the experiment is plotted as a *histogram*, where a bar is drawn at each "bin" showing the "frequency" of the result corresponding to that bin. In other words, 20 of the 50 throws had exactly one die landing with a "one" facing up, 13 had two dice, and so on.

Indeed, our expectations seem to be borne out. It often happened that one or two, or zero, dice landed that way. However, it was much rarer that three dice landed with a "one" face up, and it never happened that more than three came up. Presumably, if I threw ten or a hundred times as many handfuls, then I would have gotten a few to land with ones on five or six dice.

Let's try to predict the outcome that exactly one of the six dice lands with a "one" facing up. Let $p = 1/6$ be the probability of any one die landing with a "one" facing up. Then $q = 1 - p = 5/6$ is the probability the other five dice landing otherwise. Your first instinct might be to say that the probability of exactly one of the dice to land face up is $(1/6)^1(5/6)^5$. However, there are six equivalent ways you can get that result, since all six dice are identical. Therefore, we expect the number of throws that give us exactly one dice with a "one" facing up is the total number of throws times the probability, namely

$$N(1) = N_{\text{total}} \times \mathcal{P}(1) = 50 \times 6 \left(\frac{1}{6}\right)^1 \left(\frac{5}{6}\right)^5 = \frac{78125}{3888} \approx 20.09$$

which is pretty close to the number (20) that were observed. Of course, you can never observe exactly 20.09 occurrences because the answer has to be an integer, but, on average, this is presumably what you'd find.

Now let's predict the number of throws where exactly two dice land "successfully" with "ones" facing up. The probability of this occurrence for specific dice is now $(1/6)^2(5/6)^4$, but counting up the number of combinations that can land this way is a little trickier. We need to ask ourselves, "How many ways are there of picking two dice out of a set of six?"

Well, I have six ways to pick the first of the two, and then five ways to pick the second of the two, but I have to be aware of "double counting." That is, I could pick die #3 first and then die #5, but that's the same result as picking die #5 first and then die #3. So, the answer is $6 \cdot 5/2 = 15$. Therefore, we expect the number of successful throws to be

$$N(2) = N_{\text{total}} \times \mathcal{P}(2) = 50 \times 15 \left(\frac{1}{6}\right)^2 \left(\frac{5}{6}\right)^4 = \frac{78125}{7776} \approx 10.05$$

which again is pretty close to the number (13) that we observed.

Repeating this process for the other bins gives the black points in Figure 9.1, which I've simply joined with a straight line. It seems like we now have an understanding of how to handle probabilities of different outcomes, so we'll formalize the mathematics and then make some extensions.

9.2 Counting Permutations and Combinations

It sound be clear from our example with the dice, that we need to learn how to count efficiently. For example, we needed to know the number of ways we could select two dice from a collection of six of them, which turned out to be $6 \cdot 5/2 = 15$. We will now set up the mathematics for these kinds of calculations in general.

If you have n things arranged in a particular order, then the number possible orderings, called *permutations*, is n factorial, that is

$$n! = n(n-1)(n-2)\cdots 1$$

Try it by arranging the numbers 1, 2, and 3 in all possible orders. You have $1, 2, 3$ and $3, 1, 2$ and $2, 3, 1$ (called "cyclic permutations") and also the three orderings you get by flipping the first two of each of these, namely $2, 1, 3$ and $1, 3, 2$ and $3, 2, 1$. That's a total of $3! = 3 \cdot 2 \cdot 1 = 6$ permutations.

Now suppose you don't care about the order, but you are interested in different subsets of n things. (For example, "How many ways are there of picking two dice out of a set of six?") You now ask what is the number of *combinations* of n things taken m at a time. Well, there are n ways to pick the first thing, then $n-1$ ways to pick the second, and so on, you might write the number of combinations as

$$n(n-1)(n-2)\cdots(n-m+1)$$

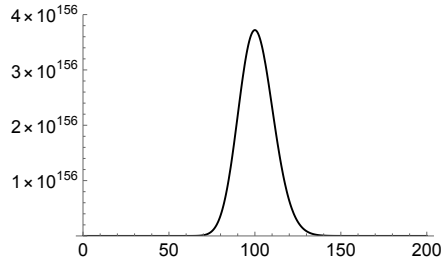


Figure 9.2: The integrand $x^n e^{-x}$ of (9.2) for $n = 100$, plotted as a function of x. Notice that the integrand peaks at $x = n = 100$, and that the shape resembles that of a Gaussian. Therefore, an approximation to $n!$ can be obtained by integrating over a Gaussian function with the appropriate mean and width.

which is a product of m factors. However, since I don't care about the order, I could pick the second first, and the third second, and the first third, and..., so I need to divide by the number of ways that I could order m possibilities, namely $m!$. Therefore, the number of combinations is

$$\binom{n}{m} \equiv \frac{n(n-1)(n-2)\cdots(n-m+1)}{m!} = \frac{n!}{m!(n-m)!} \tag{9.1}$$

This symbol is called the *Binomial Coefficient* because it tells you the coefficient of the term $p^m q^{n-m}$ in the expansion of $(p+q)^n$, namely the number of ways you can get m factors of q when you expand $(p+q)^n$.

Note that for throwing six dice, the number of combinations for one and two successes are

$$\binom{6}{1} = \frac{6!}{1!5!} = 6 \qquad \text{and} \qquad \binom{6}{2} = \frac{6!}{2!4!} = 15$$

which is just what we got in the previous section.

9.2.1 Large numbers and Stirling's approximation

Equation (9.1) is key to determining many quantities related to probabilities, and this includes almost the entire field of Statistical Mechanics.[1] However, the number of "dice" in those examples is very large, on the order of Avogadro's Number, namely $N_0 = 6.02 \times 10^{23}$. The form (9.1) is not handy for dealing with numbers like this, and we would really prefer to have some closed analytic form for $n!$.

Fortunately, we have the Γ-function (1.7) from Section 1.5.5, which we reproduce here as

$$\Gamma(n+1) = \int_0^\infty x^n e^{-x}\, dx = n! \tag{9.2}$$

for a non-negative integer $n = 0, 1, 2, 3, \ldots$. Figure 9.2 plots the integrand as a function of x for $n = 100$, and the peak position and Gaussian shape suggest that we can use what we know about Gaussian integrals to come up with an approximation for (9.2) when n is large.

[1] An excellent reference is *An Introduction to Thermal Physics*, by Daniel V. Schroeder, Oxford University Press; 1st edition (2021). This derivation follows Appendix B.3.

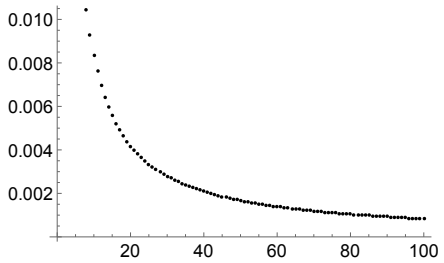


Figure 9.3: Plot of the fractional difference between $n!$ and Stirling's Approximation (9.3) for n up to 100. The approximation is rather good at $n = 100$, differing from the exact value only by about 0.1%, but the real value of Stirling's Approximation is for very large n, on the order of Avogadro's Number 6.02×10^{23}.

First let's establish the position of the peak in Figure 9.2. Since

$$\frac{d}{dx} x^n e^{-x} = n x^{n-1} e^{-x} - x^n e^{-x} = x^{n-1} e^{-x}(n - x) = 0$$

it is apparent that the Gaussian approximation peaks at $x = n$. We then define $y = x - n$ and write

$$x^n e^{-x} = e^{n \log x} e^{-x} = e^{n \log(y+n)} e^{-(y+n)} = e^{n \log[n(1+y/n)]} e^{-n} e^{-y} = e^{n \log n} e^{-n} e^{n \log(1+y/n)} e^{-y}$$

Since n is a large number, and it is clear from Figure 9.2 that $y = x - n$ is never very large, we can Taylor expand $\log(1 + y/n)$ using (2.7) to get

$$x^n e^{-x} \approx e^{n \log n} e^{-n} e^{n(y/n - y^2/2n^2)} e^{-y} = e^{n \log n} e^{-n} e^{-y^2/2n}$$

and we have confirmed that the integrand is a Gaussian in y, centered at $y = 0$. Finally, since the width of this Gaussian is on the order of $\sqrt{n} \gg 1$, we can replace the lower limit of the integral with $-\infty$, and use (1.8) to evaluate it. This results in

$$n! \approx e^{n \log n} e^{-n} \int_{-\infty}^{\infty} e^{-y^2/2n}\, dy = e^{n \log n} e^{-n} \sqrt{2\pi n} = n^n e^{-n} \sqrt{2\pi n} \tag{9.3}$$

which is known as *Stirling's Approximation*. An alternate form using the logarithm is

$$\log n! \approx n \log n - n + \frac{1}{2} \log(2\pi n)$$

where the third term is typically neglected for $n \sim 10^{23}$ in statistical mechanics.

Figure 9.3 shows the agreement between (9.3) and the exact value for $n!$, for n up to 100. The approximation is reasonably good, but gets much better for numbers n that are very large, on the order of Avogadro's Number. This is the reason it is very useful in Statistical Mechanics.

We will also find Stirling's Approximation useful when we discuss the Gaussian Probability Distribution Function, Section 9.3.3.

9.3 Probability Distributions

If a function $\mathcal{P}(m)$ gives the probability of measuring outcome m, where m is an integer, then we call $\mathcal{P}(m)$ a *discrete probability distribution function*. If the outcome is described by a continuous variable x, then $\mathcal{P}(x)\,dx$ gives the probability of measuring and outcome between x and $x + dx$, and $\mathcal{P}(x)$ is a *discrete probability distribution function*. Generically, we call $\mathcal{P}$ a *distribution*. Probability distributions are important throughout physics, from data analysis, to quantum mechanics, to statistical mechanics.

Our approach in this section will be to first write down the *binomial distribution*, which describes the situation with throwing dice. We will then discuss two extensions of the binomial distribution, namely the *Poisson distribution* and the *Gaussian distribution*, also known as the *normal distribution*.

9.3.1 The binomial distribution

We now return to our problem of throwing a handful of dice, and generalize to the question, "What is the probability that if I throw n dice, then m of them land with a one facing up?" The probability $p = 1/6$ that any one of the dice will land this way. Therefore, the probability that throwing a handful of n dice and having m of them land "successfully" with "ones" facing up is

$$\mathcal{P}_{\text{bin}}^{(1/6)}(m) = \binom{n}{m}\left(\frac{1}{6}\right)^m\left(\frac{5}{6}\right)^{n-m}$$

It is obvious how to generalize this to any situation where the probability of an individual success is p, namely

$$\mathcal{P}_{\text{bin}}^{(p)}(m) = \binom{n}{m}p^m q^{n-m} \tag{9.4}$$

where $p+q = 1$. As mentioned in Section 9.2, this is called the *binomial distribution* because it gives the term proportional to p^m of the expansion $(p+q)^n$. As such, it is clear, then, that

$$\sum_{m=0}^{n}\mathcal{P}_{\text{bin}}^{(p)}(m) = (p+q)^n = 1^n = 1$$

which must be the case, of course, since the only possible results for m are the integers from zero to n. We say that the probability distribution is *normalized*.

The black points on the right in Figure 9.1 are $N\mathcal{P}_{\text{bin}}^{(1/6)}(m)$ where m is labeled along the horizontal axis. Given a number N of dice throws, the number you expect to get would be $N\mathcal{P}_{\text{bin}}^{(1/6)}(m)$ for m dice landing with a "one" facing up. The histogram is an approximation to $\mathcal{P}_{\text{bin}}^{(1/6)}(m)$, after correcting for the normalization.

9.3.2 The Poisson distribution

The *Poisson distribution* is a limiting case of the binomial distribution, and is often taken for granted as *the* correct distribution for many problems in the statistical analysis of data. The reason is that this limiting case, namely $n \to \infty$ and $p \to 0$ with $\mu = np$ kept finite, is so often the case in physical systems. The classic case is radioactive decay, where the probability of any one radioactive nucleus decaying in a certain time interval is very small, but the number of possible decaying nuclei is very large. Another example might be the number of people in Philadelphia who might call Temple University on a Tuesday afternoon between 3pm and 4pm.

If we write (9.4) as

$$\mathcal{P}^{(p)}_{\rm bin}(m) = \frac{n!}{m!(n-m)!} p^m (1-p)^{n-m}$$

then we can see how to take the limit $n \to \infty$ and $p \to 0$ with $\mu = np$ kept finite. Firstly

$$\lim_{n\to\infty} \frac{n!}{(n-m)!} = \lim_{n\to\infty} n(n-1)\cdots(n-m+1) = n^m$$

which gives a factor $n^m p^m = \mu^m$. Now we also have

$$\lim_{n\to\infty}\lim_{p\to 0}(1-p)^{n-m} = \lim_{n\to\infty}\lim_{p\to 0}(1-p)^{n} = \lim_{p\to 0}(1-p)^{\mu/p} = \lim_{p\to 0}(1-p)^{-\mu/(-p)} = e^{-\mu}$$

Putting this together gives us the Poisson distribution, namely

$$\mathcal{P}^{(\mu)}_{\rm Poiss}(m) = \frac{\mu^m}{m!} e^{-\mu} \tag{9.5}$$

It is easy to confirm that the Poisson distribution is properly normalized, just by summing

$$\sum_{m=0}^{n} \mathcal{P}^{(\mu)}_{\rm Poiss}(m) \to \sum_{m=0}^{\infty} \mathcal{P}^{(\mu)}_{\rm Poiss}(m) = \left[\sum_{m=0}^{\infty} \frac{\mu^m}{m!}\right] e^{-\mu} = e^{\mu} e^{-\mu} = 1$$

Figure 9.4 plots (9.5) for three different values of μ. Note that for low values of μ, the probability of $m = 0$ is significant. As μ increases, the distribution peaks close to, and becomes more symmetric about, the mean.

One of the most useful properties of the Poisson distribution is that the standard deviation (Section 9.4.1) $\sigma = \sqrt{\mu}$. When you are doing an experiment and you expect the number of "successes" to be Poisson distributed, the number you observe is your best estimate of what the average out to be, so you quote a "standard error" that is the square root of the number you observe.

9.3.3 The Gaussian distribution

The Gaussian (or normal) probability distribution function is probably the most common example of a continuous variable x. It is widely used in data analysis and other fields of

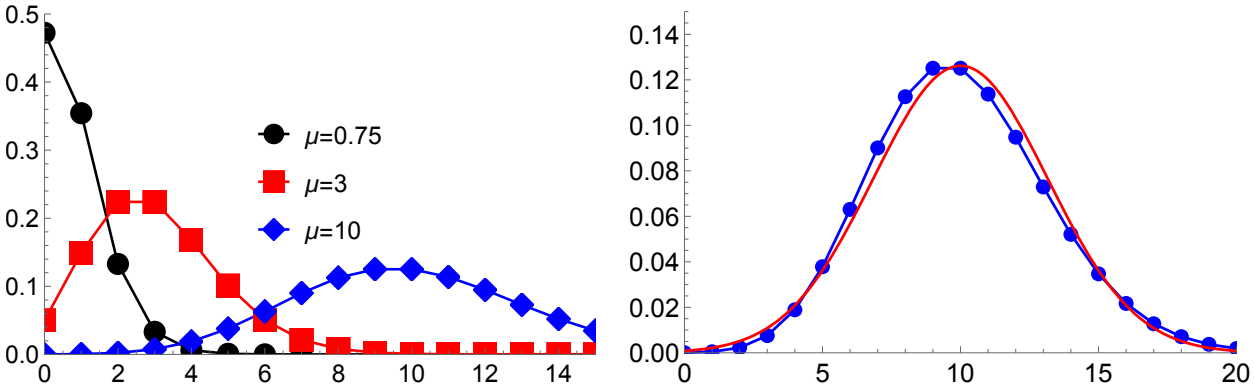


Figure 9.4: Three examples of a Poisson distribution, with three different values for the mean $\mu = 0.75, 3, 10$, are plotted on the left. On the right we reproduce the Poisson distribution for $\mu = 10$, along with the Gaussian distribution (in red) for the same μ and $\sigma = \sqrt{\mu}$.

physics, and can be derived from the binomial or Poisson distributions in the case where $m \gg 1$ and you don't stray too far from the average value. Below we will see how do this with the Poisson distribution. The result is

$$\mathcal{P}^{(\mu,\sigma)}_{\text{Gauss}}(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2} \tag{9.6}$$

It should be clear from Section 1.5.6 that this form is normalized so that

$$\int_{-\infty}^{\infty} \mathcal{P}^{(\mu,\sigma)}_{\text{Gauss}}(x)\, dx = 1$$

Let's see now how the Gaussian distribution arises from the Poisson distribution for $m \gg 1$ and $\mu \gg 1$. Take the logarithm of (9.5) and use Stirling's approximation (9.3) to write

$$\begin{aligned} \log \mathcal{P}^{(\mu)}_{\text{Poiss}}(m) &= m \log \mu - \mu - \log m! \\ &= m \log \mu - \mu - m \log m + m - \frac{1}{2}\log(2\pi) - \frac{1}{2}\log m \end{aligned}$$

We know that (9.5) has a peak when $m \approx \mu$, so it makes sense to define a variable $y \equiv m - \mu$ and expand the log around $y = 0$ using (2.7). We have

$$\begin{aligned} \log \mathcal{P}^{(\mu)}_{\text{Poiss}}(m) &= (\mu + y)\log \mu + y - \left(\mu + y + \frac{1}{2}\right)\log(\mu + y) - \frac{1}{2}\log(2\pi) \\ \text{with} \qquad \log m &= \log(y + \mu) = \log \mu + \log\left(1 + \frac{y}{\mu}\right) \approx \log \mu + \frac{y}{\mu} - \frac{y^2}{2\mu^2} \end{aligned}$$

Some algebra that is more tedious than tricky gives

$$\begin{aligned}
\log \mathcal{P}^{(\mu)}_{\rm Poiss}(m) &= y - \frac{1}{2}\log\mu - (\mu+y)\frac{y}{\mu} + (\mu+y)\frac{y^2}{2\mu^2} - \frac{y}{2\mu} - \frac{y^2}{2\mu^2} - \frac{1}{2}\log(2\pi) \\
&= \log\frac{1}{\sqrt{2\pi\mu}} - \frac{y^2}{\mu} + \frac{y^2}{2\mu} + \frac{y^3}{2\mu^2} - \frac{y}{2\mu} - \frac{y^2}{2\mu^2} \\
&= \log\frac{1}{\sqrt{2\pi\mu}} - \frac{y^2}{2\mu} + \frac{y^3}{2\mu^2} - \frac{y}{2\mu} - \frac{y^2}{2\mu^2}
\end{aligned}$$

Rewriting this in terms of $\sigma = \sqrt{\mu}$ gives us

$$\log \mathcal{P}^{(\mu)}_{\rm Poiss}(m) = \log\frac{1}{\sigma\sqrt{2\pi}} - \frac{y^2}{2\sigma^2} + \frac{1}{\sigma}\frac{y^3}{2\sigma^3} - \frac{1}{\sigma}\frac{y}{2\sigma} - \frac{1}{\sigma^2}\frac{y^2}{2\sigma^2}$$

If $y/\sigma = y/\sqrt{\mu}$ is not very large, that is if we stay close to the mean, and $\sigma = \sqrt{\mu} \gg 1$, we can neglect the last three terms compared to the second. The result is

$$\log \mathcal{P}^{(\mu)}_{\rm Poiss}(m) \to \log\frac{1}{\sigma\sqrt{2\pi}} - \frac{y^2}{2\sigma^2} \qquad \text{so} \qquad \mathcal{P}^{(\mu)}_{\rm Poiss}(m) \to \frac{1}{\sigma\sqrt{2\pi}} e^{-(m-\mu)^2/2\sigma^2}$$

which is the Gaussian approximation. Figure 9.4 also compares the Poisson distribution for $\mu = 10$ with the Gaussian distribution for the same mean and $\sigma = \sqrt{\mu}$. The agreement is obviously very good, even though $\sqrt{10}$ is not so much larger than unity. You might notice, however, that the fractional disagreement on the tails of the distribution, that is when we are far from the mean, are rather large.

9.3.4 Data histograms as approximations to distributions

I will conclude this section with a brief remark about histograms, and their role as experimental approximations to the underlying probability distributions that control.

A histogram of a quantity x is $\Delta N/\Delta x$ where ΔN is the number of events that fall into a "bin" Δx. This is what we did in the histogram for Figure 9.1, where x is the integer m. It could easily be that x was some continuous variable, though, in which case we would need to bin it.

Now, instead of multiplying the probability distribution by the total number of trials N, as in Figure 9.1, we can divide by the total number of trials. In this case, the histogram becomes an approximation to the true distribution, limited by the randomness of the finite number of trials. Then

$$\mathcal{P}(x) = \lim_{\Delta x\to 0} \frac{1}{N}\frac{\Delta N}{\Delta x} = \frac{1}{N}\frac{dN}{dx}$$

would in fact give the distribution. It is worth remembering this when using a histogram to infer a probability distribution function.

9.4 Basic Data Analysis

The term "data" is impossibly broad, so we're going to have a discussion here of simple topics confined to a simple definition of "data." It will illustrate some of the most important concepts, though, that you are likely to be concerned with during the studies of physics.

By "data" we mean generic sets of real numbers. For example, we can label them x_i and y_i for $i = 1, 2, 3, \ldots, N$. We won't make use of it here, but it is commonplace to refer to these data sets as $\underline{x}$ and $\underline{y}$ in the sense of generalized vectors, as in Section 6.2.

The arrays $\{x_i\}$ and $\{y_i\}$ are individually sets of data, and we will talk about how to calculate important quantities that collective describe them. It is also reasonable to think of these as correlated somehow, in which case we think of the data as $\{x_i, y_i\}$. In this case, it is common to have some model $y = f(x)$ which describes how the two data sets depend on each other. In many applications, the function $f(x)$ will have so-called "free parameters" which can be fit to describe the data, and there are well established techniques for finding the best fit.

9.4.1 Mean, variance, and standard deviation

A very familiar concept that you would use to describe a set of data $\{x_i\}$ is the *mean* or *average* of the values. Notations for the mean include $\langle x \rangle$ (which I will use), $\bar{x}$, and x_{avg}. You are likely well aware of the calculation of the mean of N values $\{x_i\}$, namely

$$\bar{x} = \langle x \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i \tag{9.7}$$

A less familiar concept, but at least as important as the mean, is the *variance* σ^2, which describes the "spread" of the values around the mean. It is simply the average of the square of the deviations of the values from the mean. In other words

$$\sigma^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - 2\langle x \rangle \langle x \rangle + \langle x \rangle^2 = \langle x^2 \rangle - \langle x \rangle^2 \tag{9.8}$$

The square root of the variance, that is σ, is called the *standard deviation*.

When the values $\{x_i\}$ are distributed according to some established probability distribution function, then it is possible to quantitatively predict the probability that the mean $\langle x \rangle$ is within some number of standard deviations from the correct value. A measurement of x is often reported as $\langle x \rangle \pm \sigma$, but the interpretation of the $\pm$ clearly depends on what is the appropriate distribution function. More often than not, however, people will assume it is a Gaussian distribution where $\langle x \rangle$ is a good approximation to the mean μ of the distribution.

Application to binomial, Poisson, and Gaussian distributions

If the values $\{x_i\}$ are nonnegative integers $\{m_i\}$, then it is possible that they are distributed according to the binomial or Poisson distributions.If the $\{x_i\}$ are any real numbers, however,

it might be natural to assume that are distributed according to a Gaussian. In these cases, we can calculate directly what we expect for the mean and variance. Of course, there are many other potential distribution functions, but we are only going to consider these three possibilities.

The mean value of some discrete measurement m that is distributed according to the function $\mathcal{P}(m)$ is simply the sum of the values of the measurement times the probability for getting that measurement, namely

$$\mu = \langle m \rangle = \sum_m m\mathcal{P}(m)$$

and the variance is

$$\sigma^2 = \langle (m-\mu)^2 \rangle = \langle m^2 \rangle - \langle m \rangle^2$$

We argued above that the mean of a set of numbers that follow the binomial distribution was np, where n is the number of chances of success, and p was the probability of a single success. This makes sense, because if you have n chances with each a probability p, you expect the average to be np. Let's prove this statement.

In the case the binomial distribution, we have

$$\begin{aligned}
\langle m \rangle &= \sum_{m=0}^{n} m\mathcal{P}_{\rm bin}^{(p)}(m) = \sum_{m=0}^{n} m\frac{n!}{m!(n-m)!}p^m q^{n-m} = \sum_{m=1}^{n} m\frac{n!}{m!(n-m)!}p^m q^{n-m} \\
&= \sum_{k=0}^{n-1} \frac{n!}{k!(n-k-1)!}p^{k+1}q^{n-k-1} = np\sum_{k=0}^{n-1}\frac{(n-1)!}{k!(n-1-k)!}p^k q^{n-1-k} \\
&= np\sum_{k=0}^{l}\frac{l!}{k!(l-k)!}p^k q^{l-k} = np(p+q)^l = np
\end{aligned} \tag{9.9}$$

where $l = n-1$ and $q = 1-p$. The "obvious" result is in fact correct. In order to calculate the variance, we need to evaluate

$$\begin{aligned}
\langle m^2 \rangle &= \sum_{m=0}^{n} m^2\frac{n!}{m!(n-m)!}p^m q^{n-m} = np\sum_{k=0}^{l}(k+1)\frac{l!}{k!(l-k)!}p^k q^{l-k} \\
&= np\left\{lp+1\right\} = np\left\{(n-1)p+1\right\} = n^2p^2 - np^2 + np
\end{aligned}$$

Therefore, the variance is

$$\sigma^2 = n^2p^2 - np^2 + np - (np)^2 = np(1-p) \tag{9.10}$$

for the binomial distribution (9.4).

We built the Poisson distribution based on the mean $\mu = np$ of the binomial distribution, where $n \to \infty$ and $p \to 0$. It is therefore clear that

$$\sigma^2 = \mu \tag{9.11}$$

for the Poisson distribution (9.5).

For a continuous distribution $\mathcal{P}(x)$, we integrate to get the mean and variance, that is

$$\langle x\rangle = \int_{-\infty}^{\infty} x\mathcal{P}(x)\,dx \qquad \text{and} \qquad \langle x^2\rangle = \int_{-\infty}^{\infty} x^2\mathcal{P}(x)\,dx$$

It is easy to apply these to the Gaussian distribution (9.6). Using $y = x - \mu$ we get

$$\begin{aligned}\langle x\rangle &= \int_{-\infty}^{\infty} x\mathcal{P}_{\text{Gauss}}^{(\mu,\sigma)}(x)\,dx = \frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty} xe^{-(x-\mu)^2/2\sigma^2}\,dx = \frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty}(\mu+y)e^{-y^2/2\sigma^2}\,dy \\ &= \mu\left[\frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-y^2/2\sigma^2}\,dy\right] + \frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty} ye^{-y^2/2\sigma^2}\,dy = \mu \qquad (9.12)\end{aligned}$$

where the integral in square brackets is unity because it is just the integral over the probability distribution, and the second integral is zero because the integrand is an odd function of y. Of course, this result is no surprise since we constructed the Gaussian distribution to have a peak at the mean value. In order to calculate the variance, we need

$$\frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty} x^2e^{-(x-\mu)^2/2\sigma^2}\,dx = \frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty}(\mu^2+2\mu y+y^2)e^{-y^2/2\sigma^2}\,dy$$

which we consider as three integrals. The first integral is just μ^2, and the second integral is zero because the integrand is odd. For the third integral use (1.9) to get

$$\int_{-\infty}^{\infty} y^2e^{-y^2/2\sigma^2}\,dy = \frac{1}{2}\sqrt{\pi 8\sigma^6} = \sigma^3\sqrt{2\pi}$$

Therefore, the variance of the Gaussian distribution (9.6) is

$$\mu^2 - \frac{1}{\sigma\sqrt{2\pi}}\sigma^3\sqrt{2\pi} - \mu^2 = \sigma^2 \qquad (9.13)$$

which just goes to show that we used the appropriate notation when we wrote down (9.6). Of course, we had confidence that this was the right answer when we saw how to get the Gaussian distribution from the Poisson distribution.

9.4.2 Fitting data to models

Given a set of N correlated data points $\{x_i\}$ and $\{y_i\}$, where $i = 1, 2, \ldots, N$, is very common want to "fit" a model function that describes the data as $y = f(x; a_1, a_2, \ldots, a_n)$. That is, we want to find the values of the n parameters a_j, where $j = 1, 2, \ldots, n$ so that the functional form passes as close as possible through all the data points. Typically, each data value y_i will have some uncertainty that I'll call σ_i, implying that somehow we know the standard deviation for any individual measurement of y.

If we assume (as everyone pretty much always does) that the points follow a Gaussian distribution, then the probability that data point i comes from the mean determined by the fit function is

$$\mathcal{P}_i(a_1, a_2, \ldots, a_n) = \frac{1}{\sigma_i\sqrt{2\pi}} \exp\left\{-\frac{[y_i - f(x_i; a_1, a_2, \ldots, a_n)]^2}{2\sigma_i^2}\right\}$$

The probability for a the entire set of data is therefore the product of the individual probabilities. This product is called the *likelihood*

$$\mathcal{L}(a_1, a_2, \ldots, a_n) = \prod_{i=1}^{N} \mathcal{P}_i(a_1, a_2, \ldots, a_n)$$

which is messy to write out, so I won't bother. The object of fitting the model to the data then becomes a problem of finding the values of the parameters $a_1, a_2, \ldots, a_n$ which maximize the likelihood.

Multiplying all of those exponentials together will give you a very small number for values of the parameters that are not very close to their final values. This will create headaches with computer applications that try to maximize $\mathcal{L}$, so instead we minimize the negative of the logarithm of the likelihood. That is

$$-\log \mathcal{L}(a_1, a_2, \ldots, a_n) = -\log \prod_{i=1}^{N} \left(\frac{1}{\sigma_i\sqrt{2\pi}}\right) + \frac{1}{2}\chi^2(a_1, a_2, \ldots, a_n)$$

where the first term is just some constant, and the χ^2 function is

$$\chi^2(a_1, a_2, \ldots, a_n) = \sum_{i=1}^{N} \frac{[y_i - f(x_i; a_1, a_2, \ldots, a_n)]^2}{\sigma_i^2} \tag{9.14}$$

The job of finding the best fit parameters has become a problem of finding the set of parameters which minimize $\chi^2(a_1, a_2, \ldots, a_n)$. This procedure is generally referred to as the *method of least squares.*

Given a set of data and some model function $f(x; a_1, a_2, \ldots, a_n)$, a number of tools are available for minimizing $\chi^2(a_1, a_2, \ldots, a_n)$. In MATHEMATICA, for example, the function FindFit does the job easily. Any respectable numerical library will have other options.

Fitting to linear models

The fitting problem reduces to a simple problem in linear algebra if the fitting function is strictly linear in the parameters. That is

$$f(x; a_1, a_2, \ldots, a_n) = a_1 g_1(x) + a_2 g_2(x) + \cdots + a_n g_n(x)$$

The reason this works out so nicely is that I can take the partial derivatives with respect to the a_j and set them equal to zero to minimize (9.14) and get a system of linear equations to solve for the a_j.

Let's see how this works. The χ^2 function (9.14) becomes

$$\chi^2(a_1, a_2, \ldots, a_n) = \sum_{i=1}^{N} \frac{[y_i - a_1 g_1(x_i) - a_2 g_2(x_i) - \cdots - a_n g_n(x_i)]^2}{\sigma_i^2}$$

Now take the partial derivative of this with respect to a_k and set it equal to zero.

$$-2 \sum_{i=1}^{N} \frac{[y_i - a_1 g_1(x_i) - a_2 g_2(x_i) - \cdots - a_n g_n(x_i)] g_k(x_i)}{\sigma_i^2} = 0$$

This can be rewritten as

$$\sum_{j=1}^{n} \left[\sum_{i=1}^{N} \frac{g_j(x_i) g_k(x_i)}{\sigma_i^2} \right] a_j = \sum_{i=1}^{N} \frac{y_i g_k(x_i)}{\sigma_i^2}$$

which is just a system of linear equations of the form

$$R_{kj} a_j = b_k \qquad \text{where} \qquad R_{kj} = \sum_{i=1}^{N} \frac{g_j(x_i) g_k(x_i)}{\sigma_i^2} \qquad \text{and} \qquad b_k = \sum_{i=1}^{N} \frac{y_i g_k(x_i)}{\sigma_i^2}$$

The coefficients a_j, components of the vector $\underline{a}$, are easily obtained by inverting the matrix $\underline{\underline{R}}$ and multiplying times the vector $\underline{b}$.

It would make sense here to do an example by reducing to the special case of $f(x; a, b) = ax + b$, and fitting some data. No time left in the course this semester, though.

9.5 Random Numbers and Monte Carlo Simulations

This section will occupy at most a small piece of the last class of the semester. The material really deserves a longer treatment, though.

9.5.1 Random number generation

I'm not sure how much is worth covering on random number generation. Maybe just allude to mechanisms in MATHEMATICA and other sources.

Perhaps make generating the data in Figure 9.1 a MATHEMATICA lab.

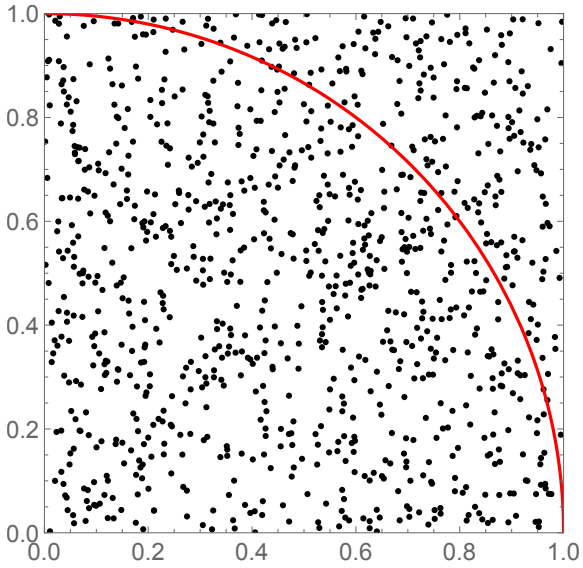


Figure 9.5: Figure showing the Monte Carlo approach to calculating π. The area inside the red circular arc is $\pi/4$. This area is estimated by generating random number pairs (x, y) inside the unit square, and then counting the number of pairs for which $x^2 + y^2 \leq 1$. An estimate of π comes from multiplying the ratio of those two numbers by four. The figures shows the positions of 1000 generated pairs, 792 of which are inside the arc, giving $\pi \approx 3.168$.

9.5.2 Integration using Monte Carlo Techniques

You can use random numbers to calculate difficult integrals numerically. These integrals could be over several different variables. The idea is to populate all of the available space defined by the variables, and then count the number of points in this space which satisfy the "area" defined by the integrand.

I will illustrate this with a simple example. The area of one quarter of the unit circle is $\pi/4$, so we can calculate π by integrating under the curve $y = f(x) = \sqrt{1 - x^2}$ over the range $0 \leq x \leq 1$. We can estimate the integral by generating a large number N of random points (x, y) over the region of the unit square defined by $0 \leq x \leq 1$ and $0 \leq y \leq 1$, and then counting up the number N_π of points that end up inside the unit circle. As N gets larger and larger, we expect to get better and better approximations to $\pi = 4N_\pi/N$.

This is illustrated in Figure 9.5, which shows the unit circle and 1000 randomly generated points. Counting up all of the points with $x^2+y^2 \leq 1$ gives 792, or $\pi \approx 4\times792/1000 = 3.168$. This is very close to $\pi = 3.142$, only 0.84% larger. Generating a large number of events gives a value for π that is closer to the right answer. Running the same code but with 10^5 generated points gives $\pi \approx 3.136$, only 0.18% from the correct value.

This discussion should include a calculation of the statistical uncertainty, but there won't be time in the last class of the term.