THE GEOMETRY OF MATHEMATICAL METHODS

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Contents

Chapter 1

Coordinates and Vectors

1.1 Polar Coordinates

Polar coordinates are useful for situations with circular symmetry in the plane. The polar coordinates (r,ϕ) of a point P are given by the distance r of P from the origin and the *angle* ϕ from the positive x-axis to P, as shown in Figure 1.1.1.

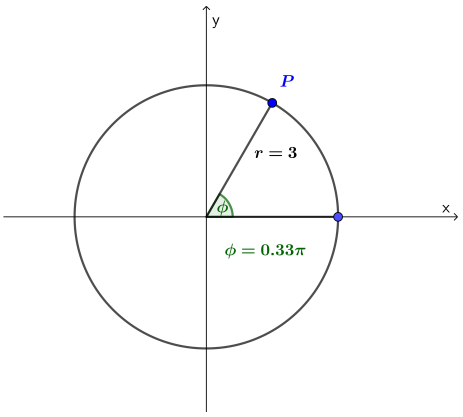


Figure 1.1.1 The construction of the polar coordinates (r,ϕ) at an arbitrary point.

Notation: When we think of the plane as a cross-section of spherical coordinates, we will use the pair (r,ϕ) for polar coordinates. When we think of the plane as a cross-section of cylindrical coordinates, we will use the pair (s,ϕ) for polar coordinates. In other references, you may also see the angle called θ instead of ϕ; we use ϕ to agree with our conventions for (cylindrical and) spherical coordinates.

It is important to remember that the angle ϕ does not measure distance; it has the wrong dimensions. Angles (in radians) are *defined* as the ratio of arclength to radius on the circle, so the arclength from the positive x-axis to P along the circle shown in the figure is $r\phi$.

1.2 Polar and Rectangular Coordinates

Section 1.1 introduced polar coordinates from scratch, without reference to rectangular coordinates. How do these coordinate systems compare?

Figure 1.2.1 redraws Figure 1.1.1 to show the values of the rectangular coordinates (x, y) as well as the values of the polar coordinates (r, ϕ) for an arbitrary point P. Using the circle definition of the trigonometric functions, we see immediately that

$$x = r\cos\phi, \tag{1.2.1}$$
$$y = r\sin\phi. \tag{1.2.2}$$

These expressions can of course be inverted, yielding

$$r = \sqrt{x^2 + y^2}, \tag{1.2.3}$$
$$\phi = \tan^{-1}\left(\frac{y}{x}\right), \tag{1.2.4}$$

which can be expressed more simply as

$$r^2 = x^2 + y^2, \tag{1.2.5}$$
$$\tan\phi = \frac{y}{x}. \tag{1.2.6}$$

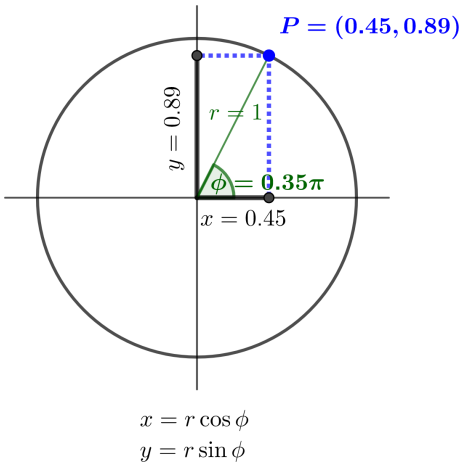


Figure 1.2.1 The construction of the polar coordinates (r,ϕ) at an arbitrary point P, showing their relationship to rectangular coordinates (x,y).

1.3 Curvilinear Coordinates

Choosing an appropriate coordinate system for a given problem is an important skill. The most frequently used coordinate system is *rectangular coordinates*, also known as *Cartesian coordinates*, after René Déscartes. One of the great advantages of rectangular coordinates is that they can be used in any number of dimensions.

In three dimensions, holding any one coordinate fixed yields a surface, which is a plane in the case of rectangular coordinates. A coordinate system can be thought of as a collection of such "constant coordinate" surfaces, and the coordinates of a given point are just the values of those constants on all the surfaces which intersect at the point. These planes are illustrated for rectangular coordinates in Figure 1.3.1.

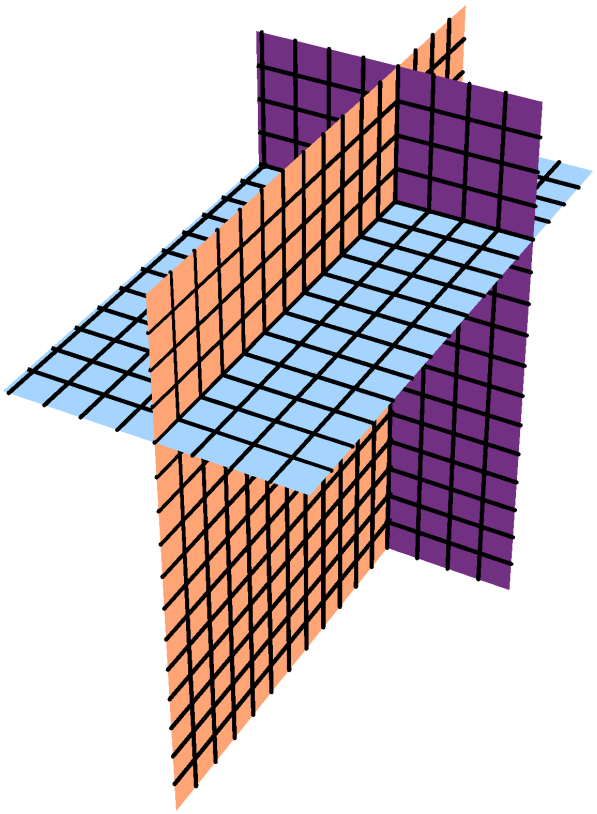


Figure 1.3.1 The coordinate planes in rectangular coordinates. On each of these planes, one of the rectangular coordinates is constant.

It is often useful, however, to use a coordinate system which shares the symmetry of a given problem — round problems should be done in round coordinates. The two standard "round" coordinate systems are *cylindrical coordinates* (s,ϕ,z), shown in Figure 1.3.2, and *spherical coordinates* (r,θ,ϕ), shown in Figure 1.3.3. Either of these coordinate systems can also be restricted to the x, y-plane, where they both reduce to *polar coordinates*. You should be aware that the standard physics conventions for spherical coordinates, used here, differ from the standard (American) math conventions; the roles of θ and ϕ are reversed. We also reserve r for the radial coordinate r in spherical coordinates, using s instead in cylindrical (and occasionally also in polar) coordinates.

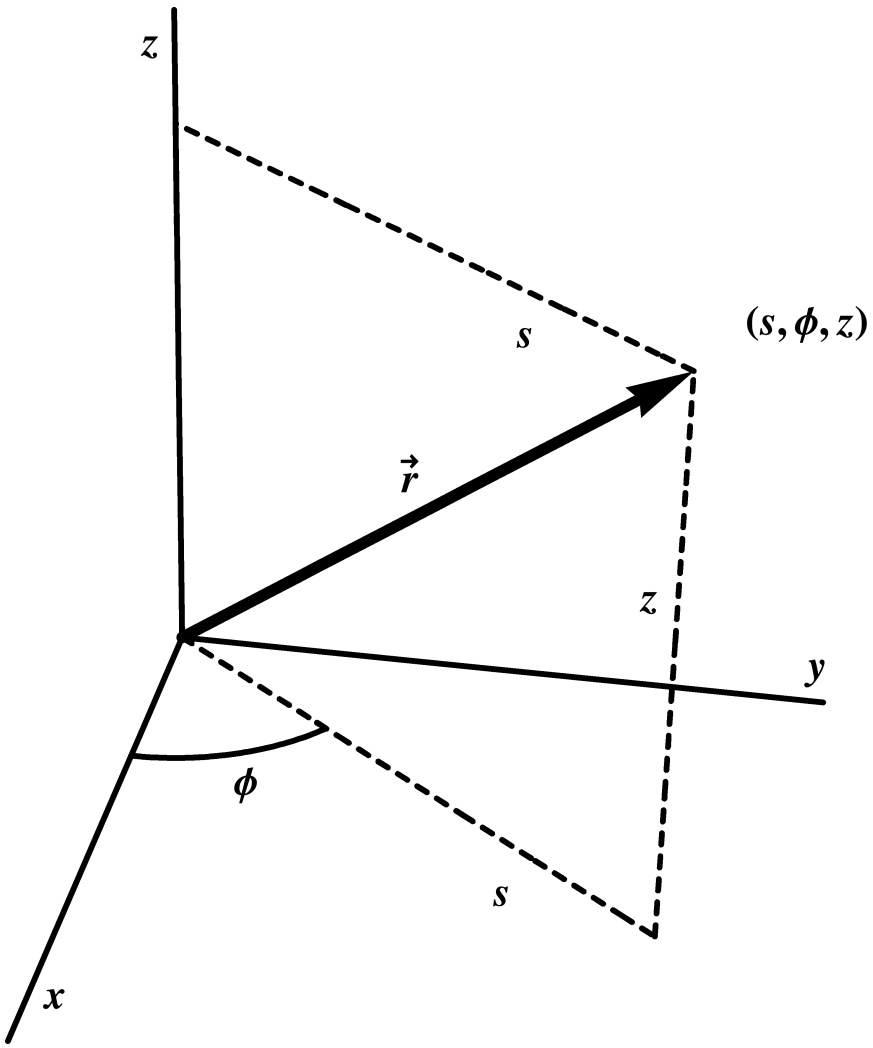


Figure 1.3.2 The geometric definition of cylindrical coordinates.

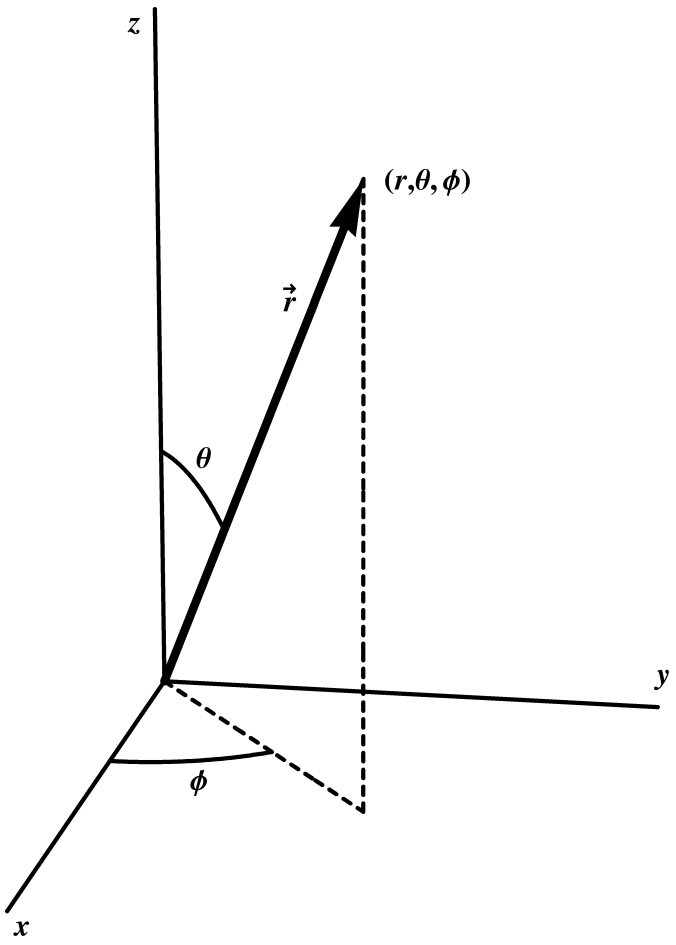


Figure 1.3.3 The geometric definition of spherical coordinates.

Sensemaking 1.3.1 Coordinate planes in curvilinear coordinates. Find the "constant coordinate" surfaces (analogous to those in Figure 1.3.4) for cylindrical and spherical coordinates.

Solution.

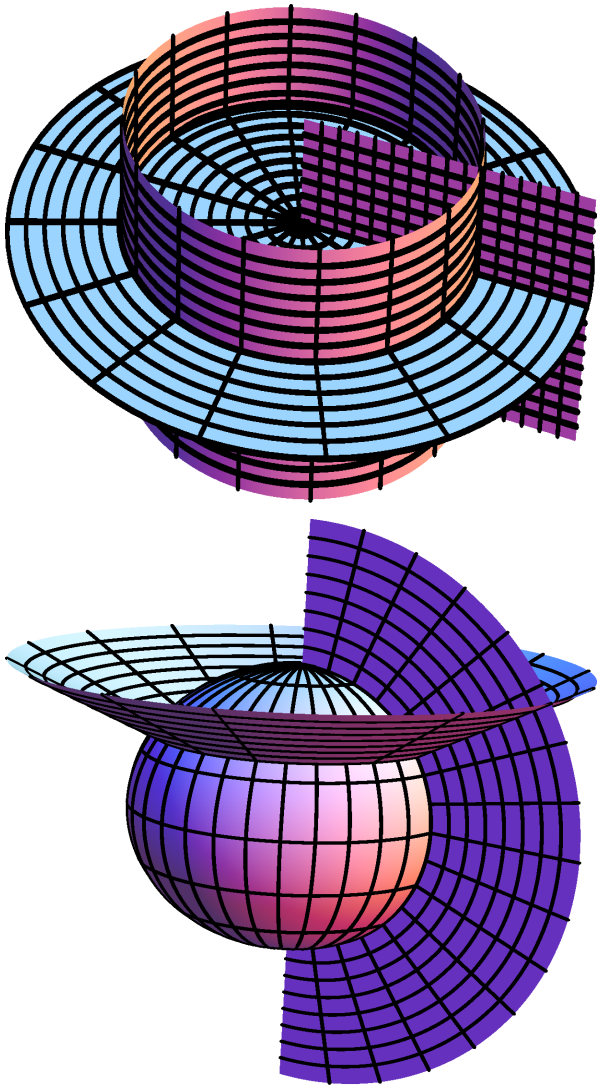


Figure 1.3.4 The coordinate planes in cylindrical and spherical coordinates.

Notation. Both of these coordinate systems reduce to polar coordinates in the x, y-plane, where $z = 0$ and $\theta = \pi/2$ if, in the cylindrical case you relabel s to the more standard r. In both cases, ϕ rather than θ is the label for the angle around the z-axis. Make sure you know which geometric angles θ and ϕ represent, rather than just memorizing their names. Whether or not you adopt the conventions used here, you should be aware that many different labels are in common use for both of these angles. In particular, you will often see the roles of θ and ϕ interchanged, particularly in mathematics texts.

Another common convention for curvilinear coordinates is to use ρ for the spherical coordinate r. We will not use ρ for the radial coordinate in spherical coordinates because we want to reserve it to represent charge or mass density. Some sources use r for both the axial distance in cylindrical coordinates and the radial distance in spherical coordinates.

1.4 Change of Coordinates

The whole point of using curvilinear coordinates is that they may be better adapted to the symmetries of a given problem. *Ideally, this means that the entire problem should be done in curvilinear coordinates, without converting between coordinate systems (although this is not always possible).* From this point of view, while it is certainly worth learning how to convert between, say, rectangular and polar coordinates, it is also worth learning how to avoid doing so as much as possible.

For completeness, the explicit transformations between these coordinate systems are given below. You should be able to use Figure 1.3.2, Figure 1.3.3, and trigonometry to verify these results. We reiterate that the conventions used here are "physicists' conventions", used by almost everyone except American mathematicians [1].

Cylindrical Coordinates:

$$\begin{aligned} x &= s\cos\phi & s^2 &= x^2 + y^2 \\ y &= s\sin\phi & \tan\phi &= y/x \\ z &= z & z &= z \end{aligned}$$

Spherical Coordinates:

$$\begin{aligned} x &= r\sin\theta\cos\phi & r^2 &= x^2 + y^2 + z^2 \\ y &= r\sin\theta\sin\phi & \tan\theta &= \sqrt{x^2 + y^2}/z \\ z &= r\cos\theta & \tan\phi &= y/x \end{aligned} \tag{1.4.1}$$

1.5 Vectors

We begin with the intuitive idea that a **vector** $\vec{w}$ is an arrow in space. Examples of vectors include the displacement from one point to another and your velocity at a point as you are moving along some path. An explicit example is shown in Figure 1.5.1.

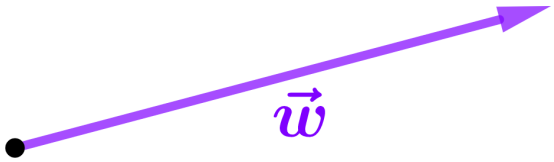


Figure 1.5.1 A vector $\vec{w}$.

What operations can we do with vectors? Two vectors can be added, using the parallelogram rule, as shown in Figure 1.5.2.

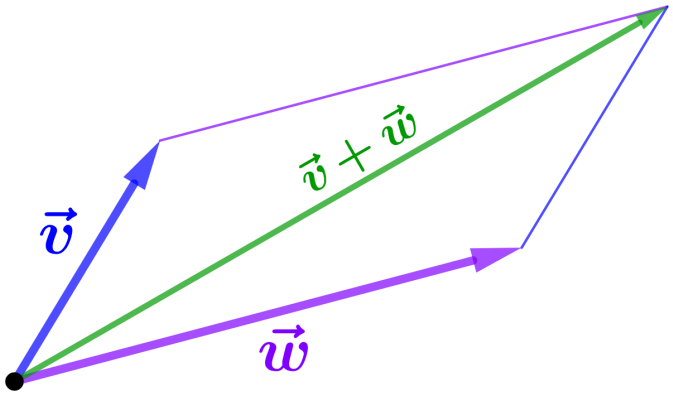


Figure 1.5.2 Adding two vectors using the parallelogram rule.

Vectors in space are anchored with their tails at a point in space, as shown by the dot in the figures. As shown in Figure 1.5.2, one adds vectors that are anchored at the same point, and the result is another vector anchored at that point.

You may have learned to add vectors by placing the tail of the second vector at the head of the first. Although that method does work in simple (flat) geometric contexts, it will fail in curved spaces (such as in general relativity).

Once we know how to add vectors, we can also rescale them. For instance, $2\vec{w} = \vec{w} + \vec{w}$. This operation can be generalized to rescale $\vec{w}$ by any real number, a process known as **scalar multiplication**.

Defining $-\vec{w}$ to point in the opposite direction from $\vec{w}$, we have

$$\vec{w} - \vec{w} = \vec{w} + (-\vec{w}) = \vec{0} \tag{1.5.1}$$

which could also have been taken as the definition of $-\vec{w}$. Thus, we can also subtract vectors, as shown in Figure 1.5.3.

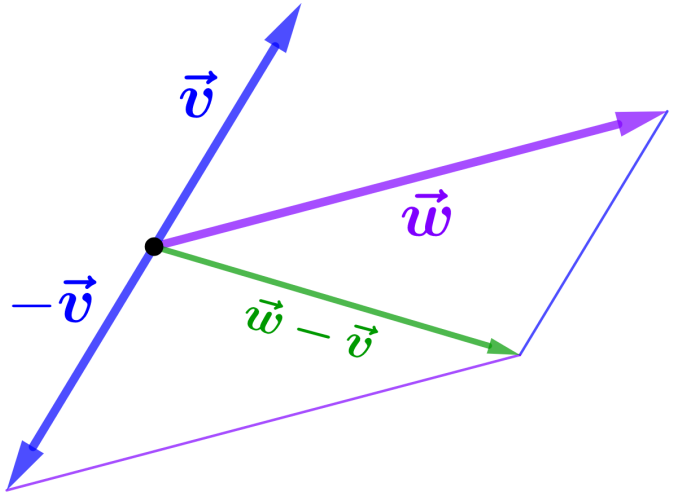


Figure 1.5.3 Subtracting two vectors using the parallelogram rule.

1.6 Bases

Intuitively, vectors in space can point up or down, right or left, and forward or backward. "Space" in this case refers to our ordinary notion of the Euclidean

geometry which we experience in our daily lives. Such vectors are said to be **three dimensional**. As a special case, some vectors are restricted to a plane, and are said to be **two dimensional**.

A two-dimensional vector, such as the one shown in Figure 1.5.1, can be expressed in terms of how much it goes "to the right" in the direction of $\vec{a}$ and how much it goes "up" in the direction of $\vec{b}$, as shown in Figure 1.6.1. This process is called **expanding** the vector in terms of the **basis vectors** $\vec{a}$ and $\vec{b}$.

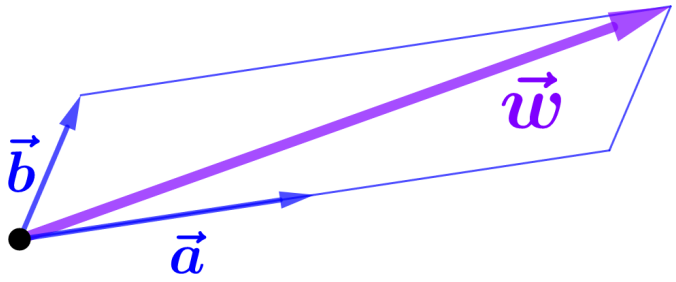


Figure 1.6.1 A two-dimensional vector $\vec{w}$, expanded in terms of a basis $\{\vec{a}, \vec{b}\}$.

There is no requirement that the basis vectors $\vec{a}$ and $\vec{b}$ used in the expansion be "perpendicular", nor that they have the same "magnitude". In fact, we do not yet know what those words mean (see Section 1.7 and Section 1.8)! Nonetheless, we can conclude from Figure 1.6.1 that $\vec{w} = 2\vec{a} + \vec{b}$.

In two dimensions, it takes two basis vectors in order to expand any vector. *Any* two linearly-independent (that is, non-parallel) vectors in the plane can be used to expand all vectors in the plane. In three dimensions, it takes a third basis vector, that is not in the plane defined by the other two, to expand any vector.

1.7 Unit Vectors

Displacement vectors have a **length**, which you can measure with a ruler. The corresponding notion for velocity vectors is the **speed** at which you are going. In either case, you can measure the angle between two such vectors using a protractor.

We use the terminology **vectors in space**, or **vectors in the plane** to refer to such geometric vectors, which have both a **magnitude** (in appropropriate units) and a **direction**. We will assume for now that all vectors are of this type, that is, that they have both direction and magnitude. [1]

The *magnitude* of $\vec{w}$ is denoted by $|\vec{w}|$, also written $||\vec{w}||$ or sometimes just as w, without an arrow on top. The magnitude of $\vec{w}$ is often casually called the "length" of $\vec{w}$, but that usage is only correct if $\vec{w}$ has dimensions of length. The displacement between two points does indeed have a length, but to talk about your speed as being the "length" of your velocity vector is confusing at best.

For example, suppose you are moving at 5 miles per hour (mph) in a roughly northeasterly direction. Your velocity $\vec{w}$ could be represented as shown in Figure 1.5.1. The magnitude of $\vec{w}$ would be 5 mph, and its direction could be specified as an angle from due north.

A **unit vector** is a vector whose magnitude is 1. Given any vector $\vec{w}$, we get a unit vector that points in the same direction as $\vec{w}$ by dividing $\vec{w}$ by its magnitude $|\vec{w}|$, that is, $\frac{\vec{w}}{|\vec{w}|}$ is a unit vector.

Unit vectors are dimensionless!

[1] Not all vectors have magnitudes!

If you divide your velocity by your speed, both measured in miles per hour, the magnitude of the result is just plain 1, *not* "1 mph". What information is left? The direction you are going. We therefore define the *direction* of a vector $\vec{\boldsymbol{w}}$ to be the unit vector in the same direction, which is just $\frac{\vec{\boldsymbol{w}}}{|\vec{\boldsymbol{w}}|}$.

As is customary in many branches of science, we will denote unit vectors with a hat, rather than an arrow. We will write the unit vectors in the x, y, and z directions as $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$, respectively. There are other common notations for these vectors. For instance, you may see $\hat{\boldsymbol{x}}$ written instead as any of $\vec{\boldsymbol{imath}}$, $\hat{\boldsymbol{\imath}}$, $\vec{\boldsymbol{a}}_x$, or $\vec{\boldsymbol{e}}_x$. You may also see the notation w and $\hat{\boldsymbol{w}}$ for the magnitude and direction, respectively, of a given vector $\vec{\boldsymbol{w}}$, so that $w = |\vec{\boldsymbol{w}}|$ and $\hat{\boldsymbol{w}} = \frac{\vec{\boldsymbol{w}}}{|\vec{\boldsymbol{w}}|}$.

Any vector $\vec{\boldsymbol{w}}$ in three dimensions can of course be expressed in terms of its components in the x, y, and z directions. For instance, we might have $\vec{\boldsymbol{w}} = 2\,\hat{\boldsymbol{x}} + 3\,\hat{\boldsymbol{y}} + 4\,\hat{\boldsymbol{z}}$. But it is important to think of vectors as arrows in space, rather than as a list of three components. While these points of view are equivalent, the former is more geometric. One of the goals of this book is to develop this geometric intuition so that it can be used in applications. It is in part for this reason that, unlike many texts, we almost always include the basis vectors $\{\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}\}$ when referring to the (Cartesian) components of a vector; we avoid writing "$\vec{\boldsymbol{w}} = \langle 2, 3, 4\rangle$". Thus, for an arbitrary vector $\vec{\boldsymbol{w}}$ with unknown (Cartesian) components, we write

$$\vec{\boldsymbol{w}} = w_x\,\hat{\boldsymbol{x}} + w_y\,\hat{\boldsymbol{y}} + w_z\,\hat{\boldsymbol{z}} \tag{1.7.1}$$

Notation. Note the use of subscripts to denote the components; these subscripts do *not* denote partial differentiation, and in fact for this reason we *never* use subscripts to denote derivatives.

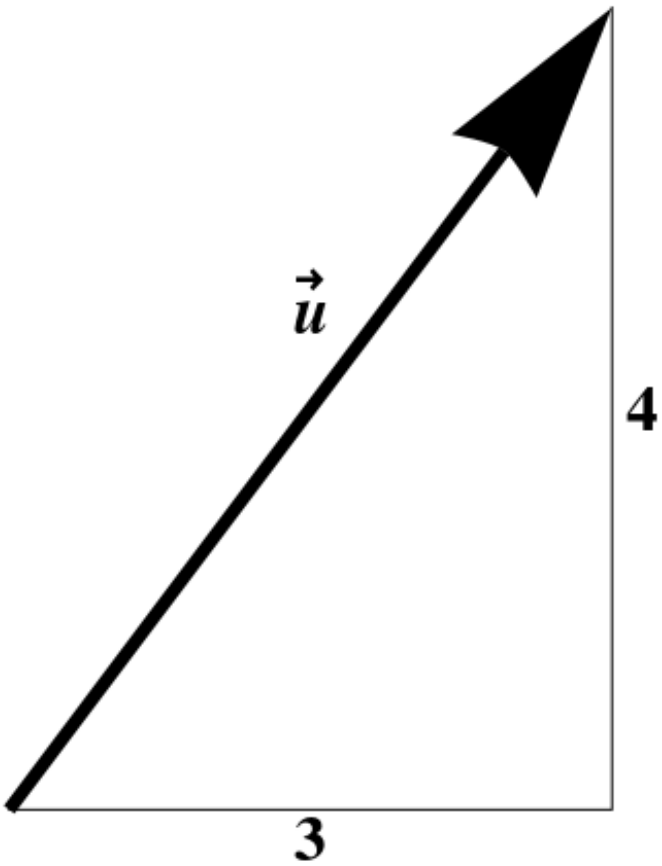


Figure 1.7.1 The vector $\vec{u}$, showing its (Cartesian) components.

For example, the components of the vector $\vec{u}$ above in Cartesian coordinates are shown in Figure 1.7.1. If $\vec{u}$ refers to your velocity, this example corresponds to your moving at 3 mph to the east and 4 mph to the north, for an overall velocity of 5 mph in the direction

$$\frac{\vec{u}}{|\vec{u}|} = \frac{3}{5}\hat{x} + \frac{4}{5}\hat{y}$$

(which could also have been specified as a compass direction).

1.8 The Dot Product

Before you read this section, you should take a few minutes to jot down everything you know about the dot product. Many students feel that if they know one representation for a concept, that is sufficient. As you will discover throughout this book, the professional scientist's ability to solve problems often comes from the ability to play off several different representations against each other.

The *geometric* definition of the dot product is given by:

$$\vec{v} \cdot \vec{w} = |\vec{v}||\vec{w}| \cos\theta \tag{1.8.1}$$

where θ is the angle between $\vec{v}$ and $\vec{w}$. Now we notice something interesting: If $\vec{v}$ is the vector along the hypotenuse of the triangle in Figure 1.8.1, then $|\vec{v}| \cos\theta$ is the projection of $\vec{v}$ onto the direction of $\vec{w}$, the other vector. Similarly,

$|\vec{w}| \cos\theta$ is the projection of $\vec{w}$ onto the direction $\vec{v}$, so the dot product is a symmetrized version of projection.

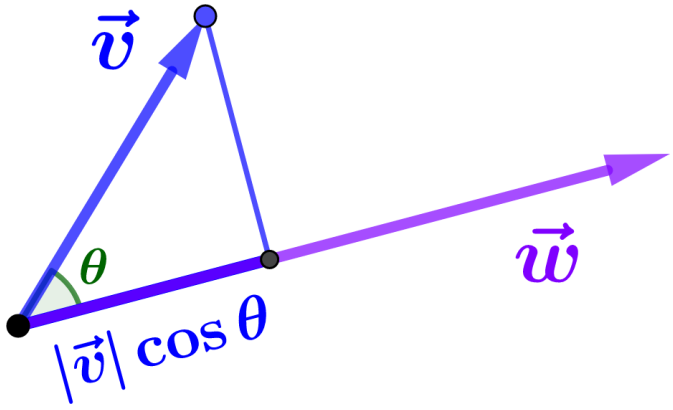


Figure 1.8.1 A projection can be found using the geometric definition of the dot product.

More precisely, in Figure 1.8.1, the length of the heavy line segment represents the component of $\vec{v}$ in the $\vec{w}$ direction. If we regard this component as the definition of the dot product of $\vec{v}$ with the *unit vector* $\frac{\vec{w}}{|\vec{w}|}$, then multiplying through by $|\vec{w}|$ and using some triangle trigonometry leads immediately to Equation (1.8.1) for the dot product of $\vec{v}$ and $\vec{w}$. (Projecting $\vec{w}$ onto $\vec{v}$ instead leads to the same result.)

Thus, the dot product is a *rescaled* projection. It is this rescaling that makes it symmetric; it doesn't matter which vector is which.

Since the angle between a vector and itself is zero, an immediate consequence of this formula is that the dot product of a vector with itself gives the square of its magnitude, that is

$$\vec{v} \cdot \vec{v} = |\vec{v}|^2. \tag{1.8.2}$$

In particular, taking the "square" of any unit vector yields 1, for example

$$\hat{x} \cdot \hat{x} = 1. \tag{1.8.3}$$

Furthermore, since $\cos\frac{\pi}{2} = 0$, it also follows immediately from the geometric definition that two (nonzero) vectors are orthogonal if and only if their dot product vanishes, that is [1]

$$\vec{v} \perp \vec{w} \iff \vec{v} \cdot \vec{w} = 0. \tag{1.8.4}$$

Because the dot product is distributive (i.e. you can "FOIL" the dot product over a sum of vectors), [2] the geometric formula Equation (1.8.1) can be used to express the dot product in terms of vector components. For example, if $\vec{v} = v_x\,\hat{x} + v_y\,\hat{y}$ and $\vec{w} = w_x\,\hat{x} + w_y\,\hat{y}$, then

$$\begin{aligned} \vec{v} \cdot \vec{w} &= (v_x\,\hat{x} + v_y\,\hat{y}) \cdot (w_x\,\hat{x} + w_y\,\hat{y}) \\ &= v_x w_x\,\hat{x} \cdot \hat{x} + v_y w_y\,\hat{y} \cdot \hat{y} + v_x w_y\,\hat{x} \cdot \hat{y} + v_y w_x\,\hat{y} \cdot \hat{x} \\ &= v_x w_x + v_y w_y \end{aligned} \tag{1.8.5}$$

[1] Since the zero vector $\vec{0}$ also satisfies this condition, it is, by definition, orthogonal to *every* other vector!

[2] There is some fine print here: we must show that the dot product is, in fact, linear in its arguments, so that it distributes over addition as claimed. This property can be established geometrically; see our online article[3].

which is often given as the *algebraic* definition of the dot product in rectangular coordinates in two dimensions. A similar formula holds in three dimensions.

A special case is the dot product of a vector with itself, which reduces to the Pythagorean theorem when written out in terms of components, for example

$$\vec{\boldsymbol{v}} \cdot \vec{\boldsymbol{v}} = |\vec{\boldsymbol{v}}|^2 = v_x^2 + v_y^2. \tag{1.8.6}$$

In the above computation we simply "multiplied out" the original expression in terms of components, then used the multiplication table

$$\begin{aligned} \hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{x}} &= 1 = \hat{\boldsymbol{y}} \cdot \hat{\boldsymbol{y}}, \\ \hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{y}} &= 0 = \hat{\boldsymbol{y}} \cdot \hat{\boldsymbol{x}}. \end{aligned}$$

Using the multiplication table of basis vectors under the dot product in this way is a useful strategy which you are encouraged to practice.

Returning to our earlier example of motion at 3 mph to the east and 4 mph to the north, we have $\vec{\boldsymbol{u}} = 3\,\hat{\boldsymbol{x}} + 4\,\hat{\boldsymbol{y}}$, so that

$$|\vec{\boldsymbol{u}}|^2 = \vec{\boldsymbol{u}} \cdot \vec{\boldsymbol{u}} = 3^2 + 4^2 = 5^2$$

and the overall speed is $|\vec{\boldsymbol{u}}| = 5$ mph as expected.

Activity 1.8.1 Combining the algebraic and geometric definitions of the dot product. Find the angle between a diagonal of a cube and one of its edges

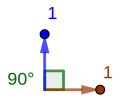
Solution. Consider the unit cube in the first octant. The vertices that we care about are at $(0,0,0), (1,0,0), (1,1,1)$. The length of the vector from the origin along the diagonal of the cube is $\sqrt{3}$ and the length of the vector along the edge is 1. By setting the dot product of these two vectors, calculated using the geometric formula Equation (1.8.1) and also the algebraic formula, equal to each other, we can solve for the cosine of the angle that we want.

$$\begin{aligned} \hat{\boldsymbol{x}} \cdot (\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}) &= |\hat{\boldsymbol{x}}|\,|(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})|\,\cos\gamma \\ 1 &= \sqrt{3}\cos\gamma \\ \cos\gamma &= \frac{1}{\sqrt{3}} \end{aligned}$$

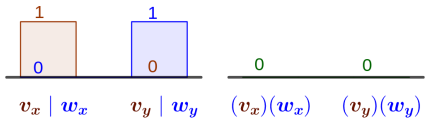
Since we know from the diagram that the angle we are looking for is less than $\frac{\pi}{2}$, choose the angle for the arccosine in the first quadrant.

1.9 Visualizing the Dot Product

The figure below shows two computations of the dot product of the given vectors, using the geometric formula (top) and the algebraic formula (bottom). The magnitude of each vector and the angle between them are shown for the first computation, whereas the second shows the horizontal and vertical components. The components are color-coded; the green bars in the algebraic representation show the products of corresponding components.



$\vec{v}_{\text{brown}} \cdot \vec{w}_{\text{blue}} = (1)(1)\cos(90°) = 0$



$\vec{v}_{\text{brown}} \cdot \vec{w}_{\text{blue}} = (v_x)(w_x) + (v_y)(w_y)$

$= (1)(0) + (0)(1) = 0 + 0 = 0$

Figure 1.9.1 Two representations of the dot product. Change the vectors by dragging their tips.

1.10 The Law of Cosines

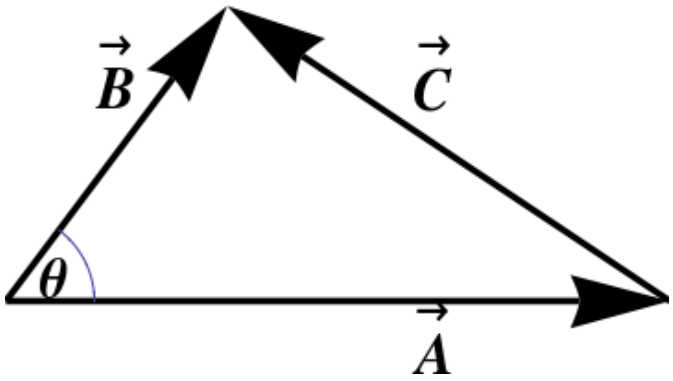


Figure 1.10.1 The Law of Cosines is just the definition of the dot product.

The definition of the dot product can be used to prove several familiar formulas. For example, consider Figure 1.10.1, in which $\vec{C} = \vec{B} - \vec{A}$. Then

$$\begin{aligned}\vec{C} \cdot \vec{C} &= (\vec{B} - \vec{A}) \cdot (\vec{B} - \vec{A}) \\ &= \vec{A} \cdot \vec{A} + \vec{B} \cdot \vec{B} - 2\,\vec{A} \cdot \vec{B}\end{aligned}$$

or equivalently

$$|\vec{C}|^2 = |\vec{A}|^2 + |\vec{B}|^2 - 2|\vec{A}||\vec{B}|\cos\theta \tag{1.10.1}$$

which is just the Law of Cosines.

1.11 Addition Formulas

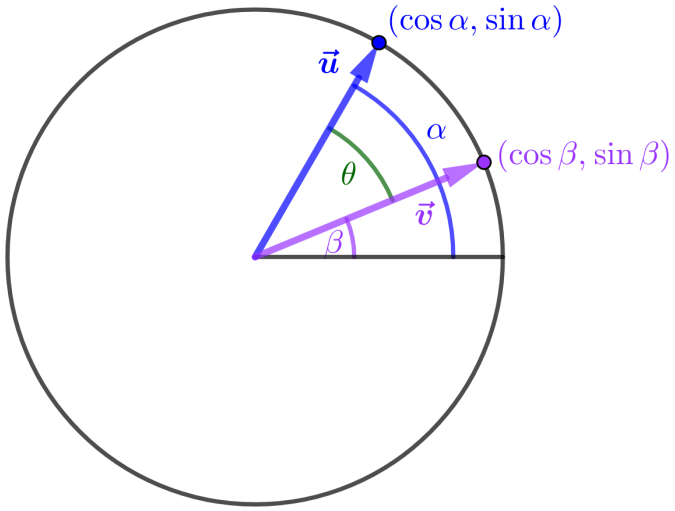


Figure 1.11.1 The derivation of the trigonometric addition formulas using the definition of the dot product.

The definition of the dot product was used in Section 1.10 to provide a straightforward derivation of the Law of Cosines. A similar argument can be used to derive the addition formulas for trigonometric functions, starting with cosine.

Consider the unit vectors $\vec{\boldsymbol{u}}$ and $\vec{\boldsymbol{v}}$, shown on the unit circle in Figure 1.11.1. Their components are given by the coordinates of their endpoints on the unit circle, so elementary circle trigonometry implies that

$$\vec{\boldsymbol{u}} = \cos\alpha\,\hat{\boldsymbol{x}} + \sin\alpha\,\hat{\boldsymbol{y}}, \tag{1.11.1}$$

$$\vec{\boldsymbol{v}} = \cos\beta\,\hat{\boldsymbol{y}} + \sin\beta\,\hat{\boldsymbol{y}}. \tag{1.11.2}$$

Computing $\vec{\boldsymbol{u}} \cdot \vec{\boldsymbol{v}}$ algebraically, we obtain

$$\vec{\boldsymbol{u}} \cdot \vec{\boldsymbol{v}} = \cos\alpha\,\cos\beta + \sin\alpha\,\sin\beta. \tag{1.11.3}$$

On the other hand, since the angle θ between $\vec{\boldsymbol{u}}$ and $\vec{\boldsymbol{v}}$ is clearly $\beta - \alpha$, and since $\vec{\boldsymbol{u}}$ and $\vec{\boldsymbol{v}}$ are unit vectors, the geometric formula for the dot product yields

$$\vec{\boldsymbol{u}} \cdot \vec{\boldsymbol{v}} = |\vec{\boldsymbol{u}}|\,|\vec{\boldsymbol{v}}|\,\cos\theta = \cos(\alpha - \beta). \tag{1.11.4}$$

Equating these two expressions for the dot product yields

$$\cos(\alpha - \beta) = \cos\alpha\,\cos\beta - \sin\alpha\,\sin\beta \tag{1.11.5}$$

which is the addition formula for cosine.

Addition formulas for the remaining trigonometric functions can be found as usual, using relations such as $\sin\theta = \cos(\frac{\pi}{2} - \theta)$ and $\tan\theta = \frac{\sin\theta}{\cos\theta}$.

1.12 Orthonormal Basis Vectors

In (1.7.1), we expressed an arbitrary vector $\vec{\boldsymbol{w}}$ in three dimensions in terms of the rectangular basis $\{\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}\}$. We have adopted the physics convention of writing unit vectors (i.e. vectors with magnitude one) with hats, rather than with arrows. You may find this to be a useful mnemonic.

An older, but still popular, convention is to call these basis vectors $\{\hat{\boldsymbol{\imath}}, \hat{\boldsymbol{\jmath}}, \hat{\boldsymbol{k}}\}$, respectively. This convention is a historical hangover from attempts to describe electrodynamics with quaternions in the late 1800's!

When using curvilinear coordinates (see Section 1.3) it is often useful to expand the vector in terms of unit vectors associated with the curvilinear coordinates instead of the rectangular basis vectors above. For example, just as $\hat{\boldsymbol{x}}$ points in the direction in which x increases, $\hat{\boldsymbol{r}}$ is defined to be the unit vector pointing in the direction of increasing r (with the other coordinates held fixed). [1]

In general, a basis vector of the form $\widehat{coordinate}$ is the unit vector that points in the direction in which *coordinate* is changing. However, unlike the rectangular basis vectors, these vector fields vary from point to point.

Activity 1.12.1 Curvilinear Basis Vectors. Imagine that the origin of coordinates is behind you in the corner of the room you are sitting in, on the floor, on the left-hand side. Think of your right shoulder as a point in space. You should use your right arm to represent, successively, each of the basis vectors $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$ in rectangular coordinates, $\hat{\boldsymbol{s}}$, $\hat{\boldsymbol{\phi}}$, and $\hat{\boldsymbol{z}}$ in cylindrical coordinates and $\hat{\boldsymbol{r}}$, $\hat{\boldsymbol{\theta}}$, and $\hat{\boldsymbol{\phi}}$ in spherical coordinates.

Hint.

[1] In some of our past materials, we have used a convention in which r and $\hat{\boldsymbol{r}}$ refer to geometrically different quantities in cylindrical than in spherical coordinates. If it is not obvious from the context (it usually is), care must be taken to specify in which coordinate system one is working.

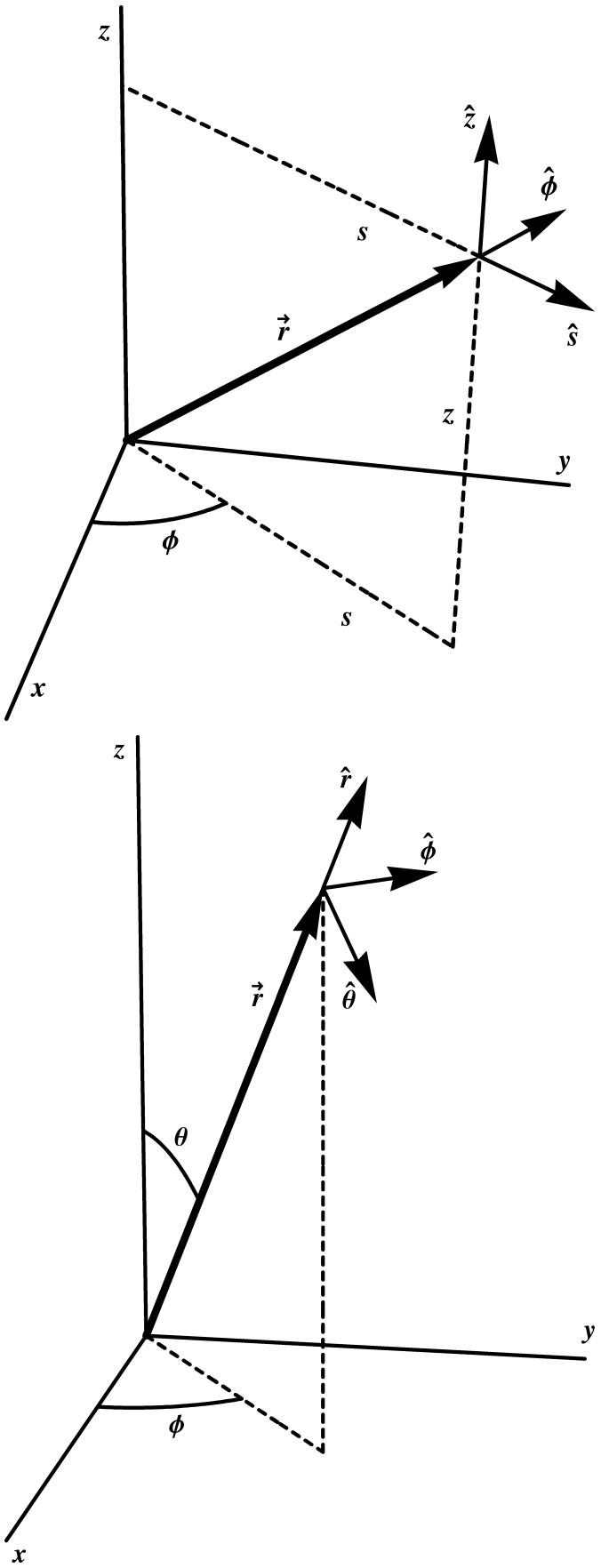


Figure 1.12.1 The definition of cylindrical and spherical coordinates, showing the associated basis vectors.

In this activity, you should have learned the following things.

1. Figure 1.12.1 shows the directions that you should have pointed if you were standing at a particular position in the room. Make sure that the directions in which you pointed agree with the directions shown in the figure. In particular, $\hat{\boldsymbol{\theta}}$ should point generally downward (for $z > 0$) since θ is measured from the positive z-axis.
2. The basis vectors are vectors, that is, they are *straight* arrows in space, even when they correspond to coordinates that are angles. Your arm should therefore have been straight, no matter which basis vector you were representing.
3. Although the basis vectors that correspond to rectangular coordinates x, y, and z are constants, and point in the same direction at each point in space, most of the basis vectors that correspond to cylindrical and spherical coordinates point in different directions at different points in space. Figure 1.12.2 shows the construction of the polar (or cylindrical) basis vectors $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{\phi}}$ at a particular point in a way that details how the direction of these vectors depends on the coordinate ϕ of the point.
4. The basis vectors adapted to a single coordinate form a simple example of the geometrical notion of a *vector field*, that is, a vector at every point in space, see Section 1.20. As an example, Figure 1.20.1 shows these basis vector fields in polar coordinates.

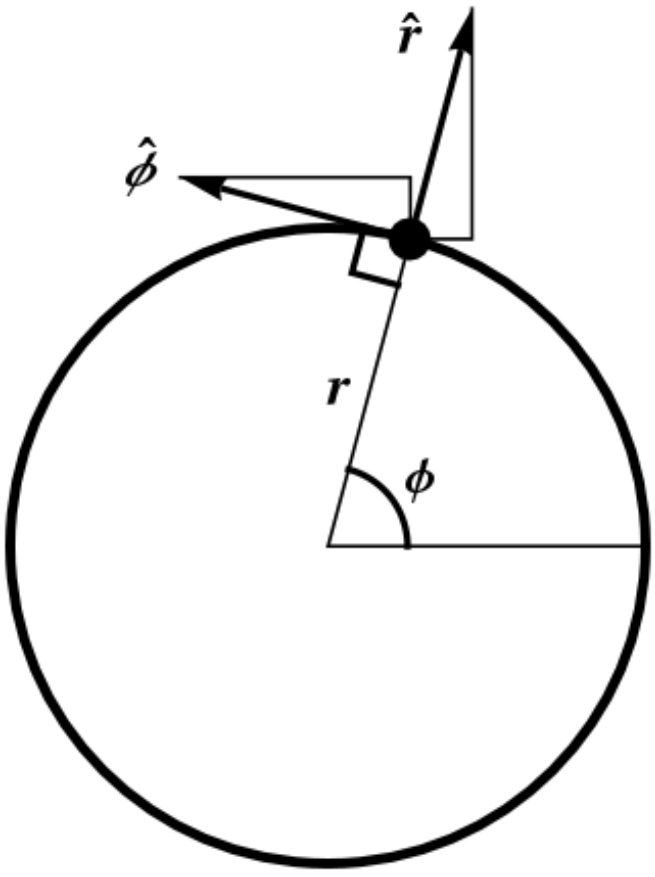


Figure 1.12.2 The construction of the polar basis $\{\hat{\boldsymbol{r}}, \hat{\boldsymbol{\phi}}\}$ at a specific point in the plane.

1.13 Polar basis vectors

Curvilinear basis vectors are *vector fields*, that is, they depend on the point where they are located. So the relationship between two such bases also depends on location.

Activity 1.13.1 At the point P shown below, first draw the rectangular basis vectors $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$, then draw the polar basis vectors $\hat{\boldsymbol{s}}$ and $\hat{\boldsymbol{\phi}}$. Finally, use your drawing to work out the relationship between these basis vectors. Make sure that your formula works for every quadrant. Note: You can move the point P in the figures below.

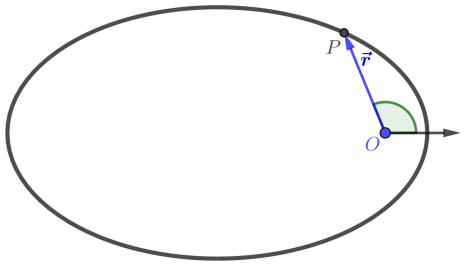


Figure 1.13.1 Polar Coordinates.

Hint.

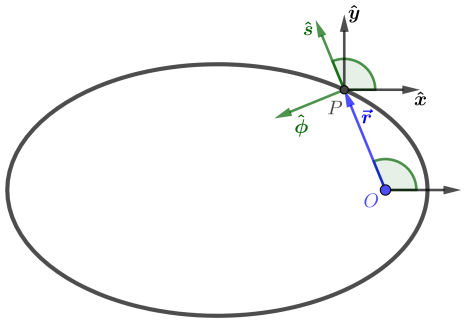


Figure 1.13.2 Draw the polar basis vectors at the point P.

1.14 Orthonormality of Basis Vectors

In this book we will only work with *orthonormal coordinates*, such as rectangular, cylindrical, or spherical coordinates. Each such coordinate system is called *orthogonal* because the basis vectors adapted to the three coordinates point in mutually orthogonal directions, i.e. the basis vectors adapted to a particular coordinate system are perpendicular to each other at every point. In particular,

$$\hat{\boldsymbol{s}} \cdot \hat{\boldsymbol{\phi}} = \hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{z}} = \hat{\boldsymbol{z}} \cdot \hat{\boldsymbol{s}} = 0 \qquad \text{(cylindrical)},$$
$$\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\theta}} \cdot \hat{\boldsymbol{\phi}} = \hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{r}} = 0 \qquad \text{(spherical)}.$$

Figure 1.12.2 shows this orthogonality in the case of polar basis vectors.

We can also choose the basis vectors to be normalized, i.e. they are unit vectors:

$$\hat{\boldsymbol{s}} \cdot \hat{\boldsymbol{s}} = \hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{\phi}} = \hat{\boldsymbol{z}} \cdot \hat{\boldsymbol{z}} = 1 \qquad \text{(cylindrical)},$$
$$\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{r}} = \hat{\boldsymbol{\theta}} \cdot \hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{\phi}} = 1 \qquad \text{(spherical)}.$$

A basis with both of the orthogonal property and the normalization property is called *orthonormal*.

Arbitrary vectors can be expanded in terms of a basis; this is why they are called *basis vectors* to begin with. The expansion of an arbitrary vector $\vec{\boldsymbol{v}}$ in terms of its components in the three most common orthonormal coordinate systems is given by:

$$\begin{aligned}\vec{\boldsymbol{v}} &= v_x\,\hat{\boldsymbol{x}} + v_y\,\hat{\boldsymbol{y}} + v_z\,\hat{\boldsymbol{z}} && \text{(rectangular)},\\ &= v_s\,\hat{\boldsymbol{s}} + v_\phi\,\hat{\boldsymbol{\phi}} + v_z\,\hat{\boldsymbol{z}} && \text{(cylindrical)},\\ &= v_r\,\hat{\boldsymbol{r}} + v_\theta\,\hat{\boldsymbol{\theta}} + v_\phi\,\hat{\boldsymbol{\phi}} && \text{(spherical)}.\end{aligned}$$

It is straightforward to find the components of an arbitrary vector field $\vec{\boldsymbol{v}}$ in terms of an orthonormal basis. Since the vectors in an orthonormal basis are mutually orthogonal, it is just a matter of using the dot product to figure out how much of $\vec{\boldsymbol{v}}$ points in each of those directions.

Activity 1.14.1 Finding Coefficients. Find the $\hat{\boldsymbol{\phi}}$-component of the vector $\vec{\boldsymbol{v}}$.

Solution. Since the basis is orthonormal, it is straightforward to compute the components algebraically. For example,

$$\vec{\boldsymbol{v}} = v_s\,\hat{\boldsymbol{s}} + v_\phi\,\hat{\boldsymbol{\phi}} + v_z\,\hat{\boldsymbol{z}}, \tag{1.14.1}$$

$$\begin{aligned}\hat{\boldsymbol{\phi}}\cdot\vec{\boldsymbol{v}} &= \hat{\boldsymbol{\phi}}\cdot\left(v_s\,\hat{\boldsymbol{s}} + v_\phi\,\hat{\boldsymbol{\phi}} + v_z\,\hat{\boldsymbol{z}}\right)\\ &= \left(\hat{\boldsymbol{\phi}}\cdot v_s\,\hat{\boldsymbol{s}} + \hat{\boldsymbol{\phi}}\cdot v_\phi\,\hat{\boldsymbol{\phi}} + \hat{\boldsymbol{\phi}}\cdot v_z\,\hat{\boldsymbol{z}}\right)\\ &= \left(0 + v_\phi\,1 + 0\right), \qquad (1.14.2)\\ \Rightarrow v_\phi &= \hat{\boldsymbol{\phi}}\cdot\vec{\boldsymbol{v}}, \qquad (1.14.3)\end{aligned}$$

with similar expressions holding for the other components.

Of course, this calculation is overkill if you already have the vector $\vec{\boldsymbol{v}}$ visibly decomposed as in Equation (1.14.1). In that case, you should just read off the coefficient of $\hat{\boldsymbol{\phi}}$. This method becomes useful if the expansion in Equation (1.14.1) is algebraically hidden in some way.

You can also find coefficients geometrically:

$$\begin{aligned}v_\phi &= \hat{\boldsymbol{\phi}}\cdot\vec{\boldsymbol{v}}\\ &= |\hat{\boldsymbol{\phi}}|\,|\vec{\boldsymbol{v}}|\,\cos\alpha\end{aligned}$$

where α is the angle between $\vec{\boldsymbol{v}}$ and $\hat{\boldsymbol{\phi}}$ and $|\hat{\boldsymbol{\phi}}| = 1$.

In situations with high symmetry, many physical quantities may be simpler to understand or interpret if they are written in terms of curvilinear basis vectors. However, you must be *very* careful anytime you are adding or subtracting (or integrating, which is just a continuous form of adding) vectors expressed in curvilinear basis vectors.

Warning 1.14.1 Never add or integrate expressions involving curvilinear basis vectors at more than one point. When using basis vectors adapted to curvilinear coordinates in sums and differences (including integrals), it is essential to remember that these basis vectors are not constant. For example, if you try to add two vectors that are expanded in terms of the basis vectors appropriate to two different points, e.g. $\{\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{\theta}}_1, \hat{\boldsymbol{\phi}}_1\}$ and $\{\hat{\boldsymbol{r}}_2, \hat{\boldsymbol{\theta}}_2, \hat{\boldsymbol{\phi}}_2\}$, you cannot simply add the components:

$$\vec{\boldsymbol{v}}_1 + \vec{\boldsymbol{w}}_2 = (v_r\hat{\boldsymbol{r}}_1 + v_\theta\hat{\boldsymbol{\theta}}_1 + v_\phi\hat{\boldsymbol{\phi}}_1) + (w_r\hat{\boldsymbol{r}}_2 + w_\theta\hat{\boldsymbol{\theta}}_2 + w_\phi\hat{\boldsymbol{\phi}}_2)$$

$$\neq (v_r + w_r)\hat{\boldsymbol{r}} + (v_\theta + w_\theta)\hat{\boldsymbol{\theta}} + (v_\phi + w_\phi)\hat{\boldsymbol{\phi}}$$

The last line is not correct because $\{\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{\theta}}_1, \hat{\boldsymbol{\phi}}_1\} \neq \{\hat{\boldsymbol{r}}_2, \hat{\boldsymbol{\theta}}_2, \hat{\boldsymbol{\phi}}_2\}$, so that the coefficients of the basis vectors *cannot* be factored out. The only way out of this dilemma is to rewrite the curvilinear basis vectors in terms of rectangular basis vectors. Since rectangular basis vectors do not change from point to point, they *can* be factored out of the relevant expressions.

Similarly, later in this text, when we discuss taking various derivatives of vector fields, we will need to show how to take the derivatives of these curvilinear basis vectors.

1.15 The Position Vector

The **position vector** $\vec{\boldsymbol{r}}$ is the displacement vector that points from the origin to a given point P, as shown in Figure 1.15.1. It is important to note that the position vector depends not only on the given point, but also on the choice of origin.

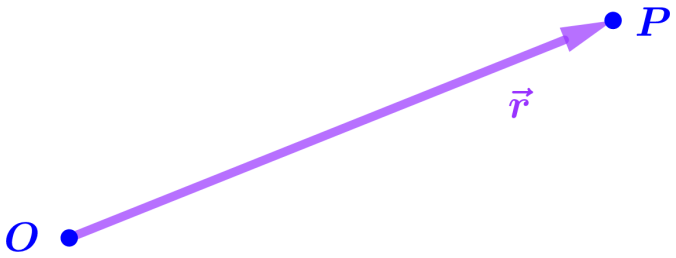


Figure 1.15.1 The position vector corresponding to the point P.

As with any vector, we can express the position vector in terms of a basis. In rectangular coordinates, the position vector is given by

$$\begin{aligned}\vec{\boldsymbol{r}} &= r_x\,\hat{\boldsymbol{x}} + r_y\,\hat{\boldsymbol{y}} + r_z\,\hat{\boldsymbol{z}} \\ &= x\,\hat{\boldsymbol{x}} + y\,\hat{\boldsymbol{y}} + z\,\hat{\boldsymbol{z}}\end{aligned} \tag{1.15.1}$$

since the components $\{r_x, r_y, r_z\}$ of the position vector are just the rectangular coordinates (x, y, z) of the point \$P\$.

1.16 The Position Vector in Curvilinear Coordinates

The position vector is easier to write algebraically in rectangular coordinates than it is to think about:

$$\vec{\boldsymbol{r}} = x\,\hat{\boldsymbol{x}} + y\,\hat{\boldsymbol{y}} + z\,\hat{\boldsymbol{z}}. \tag{1.16.1}$$

What happens in curvilinear coordinates? Naive pattern matching with (1.16.1) might lead you to believe that the position vector in spherical coordinates is given by:

$$\vec{\boldsymbol{r}} = r\,\hat{\boldsymbol{r}} + \theta\,\hat{\boldsymbol{\theta}} + \phi\,\hat{\boldsymbol{\phi}} \qquad \text{(incorrect)}. \tag{1.16.2}$$

However, if you try to follow this equation as a literal set of instructions, then the instructions say "first travel the distance r in the $\hat{\boldsymbol{r}}$ direction (which already gets you to where you want to go) and then from there, travel the distance θ (which is an angle, not a distance) in the $\hat{\boldsymbol{\theta}}$ direction and then from there,

travel the distance ϕ (which is also an angle, not a distance) in the $\hat{\boldsymbol{\phi}}$ direction." These directions are clearly incorrect; we should have stopped after the first step. In spherical coordinates, the position vector is given by:

$$\vec{\boldsymbol{r}} = r\,\hat{\boldsymbol{r}} \qquad \text{(correct)}. \tag{1.16.3}$$

Don't forget that the position vector depends on the point P at which you are looking. However, if you try to write the position vector $\vec{\boldsymbol{r}}(P)$ for a particular point P in spherical coordinates, and you think of the tail of the position vector as "attached" to the origin, then you have a problem. It is not clear which $\hat{\boldsymbol{r}}$, $\hat{\boldsymbol{\theta}}$, and $\hat{\boldsymbol{\phi}}$ you should use. The resolution to this dilemma, of course, is to think of the tail as "attached" to the point P and to use the $\hat{\boldsymbol{r}}$, $\hat{\boldsymbol{\theta}}$, and $\hat{\boldsymbol{\phi}}$ at P. We can use a subscript P to denote this particular choice of basis vectors $\hat{\boldsymbol{r}}_P$, $\hat{\boldsymbol{\theta}}_P$, and $\hat{\boldsymbol{\phi}}_P$. If you are trying to use the position vector to tell someone how to get to P from the origin and you try to use curvilinear coordinate basis vectors, it turns out to be somewhat tricky. As discussed above, the process boils down to facing in the correct direction ($\hat{\boldsymbol{r}}_P$), then going the correct distance (r), so that

$$\vec{\boldsymbol{r}}(P) = r\,\hat{\boldsymbol{r}}_P. \tag{1.16.4}$$

If you are trying to use the position vector to tell someone how to get to P from the origin and you try to use curvilinear coordinate basis vectors, then they have to know where P is in order to understand your description in terms of the basis vectors, $\hat{\boldsymbol{r}}_P$, $\hat{\boldsymbol{\theta}}_P$, and $\hat{\boldsymbol{\phi}}_P$, at P!

You should try to use a similar process to find the position vector in cylindrical coordinates.

1.17 The Position Vector as a Vector Field

The position vector is a unique and very peculiar beast.

Consider the electric field due to a point charge. It consists of a vector at each point in space, and is best represented by a vector graph where the tail of each vector is "attached" to the point in space at which the electric field is evaluated. Such vector graphs represent **vector fields**, as discussed more fully in Section 1.20.

On the other hand, the position vector $\vec{\boldsymbol{r}}$ corresponding to a particular point P in space points from an arbitrary but specific, fixed origin to the point P, i.e. its tail is at the origin. If we now let the point P vary all over space, then the position vector becomes a vector field, which we could write as $\vec{\boldsymbol{r}}(P)$. There is one vector for each point in space, just as for an ordinary vector field, but now each vector is most naturally represented with its tail at the origin and its *head* "attached" to the point in space at which the position vector field is being evaluated. See Figure 1.17.1.

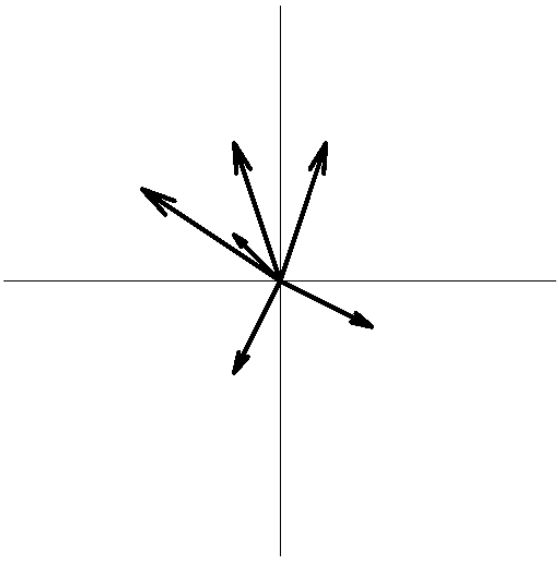


Figure 1.17.1 The position vectors corresponding to several arbitrary points P, with the tails of the vectors "attached" to the origin.

You certainly *can* represent the position vector by "moving" the tail of each vector in the vector field to the point P and then making the vector point away from the origin and have the magnitude of the vector be the distance of the point P from the origin; see Figure 1.17.2. However, it may make your head hurt to think about it this way if you continue to think of the position vector as telling you, geometrically, how to get from the origin to the point P.

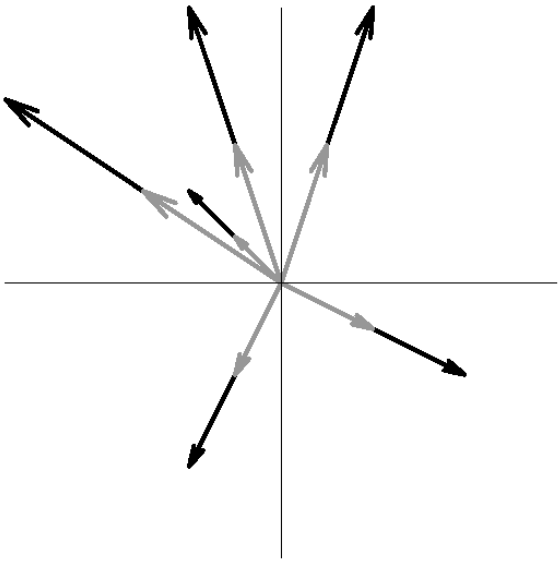


Figure 1.17.2 The same position vectors as in Figure 1.3.1, but now with the tails of the vectors "moved" to the relevant points P.

1.18 The Distance Formula

If you want to find the distance between two objects in the real world, you measure the distance with a ruler (unless you are an astrophysicist and the distances are too large or you are a particle physicist and the distances are too small!). But, if you are a theoretician and you want to put the distance into a formula, things are not quite so simple. First, you need information about where the two objects are. Perhaps you know coordinates of the two points in some rectangular coordinate system, say (x_1, y_1, z_1) and (x_2, y_2, z_2). Then the three-dimensional version of the Pythagorean theorem shows that the distance between the objects is

$$\begin{aligned} \text{distance} &= \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2} \\ &= \sqrt{(\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2}. \end{aligned} \tag{1.18.1}$$

Sensemaking 1.18.1 The Pythagorean Theorem in 3 Dimensions. Use the Pythagorean Theorem in 2 dimensions to derive formula (1.18.1) for the Pythagorean Theorem in 3 dimensions.

Hint. To determine the length of the heavy red line, first project it into the xy-plane. Use the Pythagorean theorem twice, first on the (projected) red triangle and then on the (vertical) blue triangle in Figure 1.18.1.

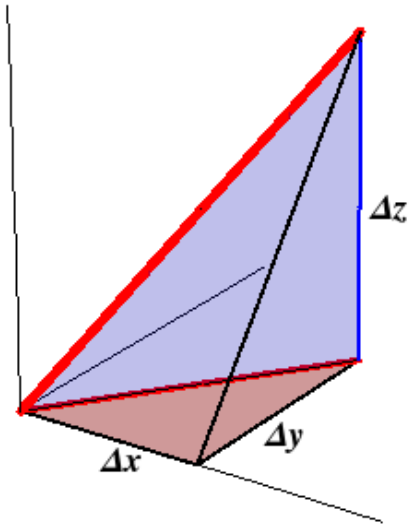


Figure 1.18.1 The Pythagorean theorem can be extended to three dimensions.

But what if the theoretician wants to use a coordinate independent expression in her formulas. How does she say where the objects are? By using the position vectors $\vec{r}_1$ and $\vec{r}_2$. Figure 1.18.2 shows the position vectors $\vec{r}_1$ and $\vec{r}_2$ for two objects, as well as their difference, $\vec{r}_2 - \vec{r}_1$. The magnitude of this latter vector is the distance between the two objects. The magnitude property of the dot product says that the magnitude of any vector is the square root of the dot product of the vector with itself. Therefore, the distance between the two objects, in coordinate independent form is:

$$\text{distance} = |\vec{r}_2 - \vec{r}_1| = \sqrt{(\vec{r}_2 - \vec{r}_1) \cdot (\vec{r}_2 - \vec{r}_1)}. \tag{1.18.2}$$

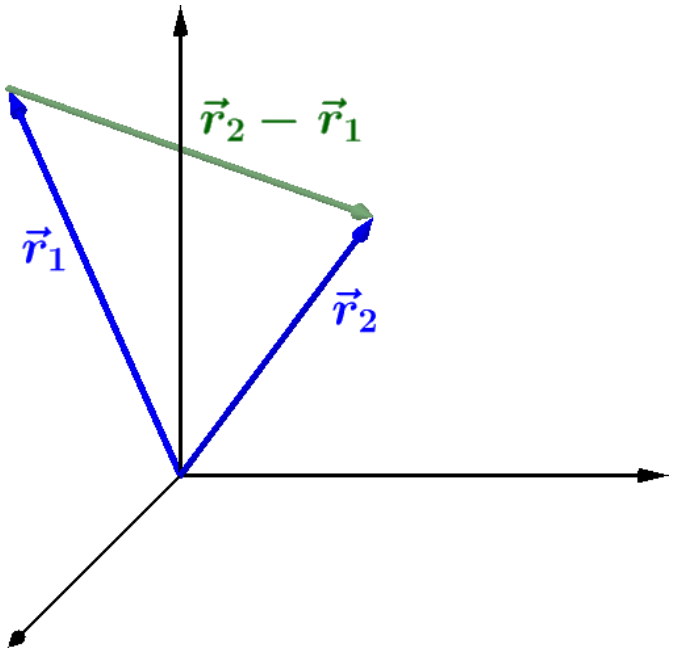


Figure 1.18.2 The position vectors $\vec{r}_1$ and $\vec{r}_2$ for two objects, and their difference, $\vec{r}_2 - \vec{r}_1$. The magnitude of the difference is the distance between the two objects.

Sensemaking 1.18.2 Two Distance Formulas. Show that the two equations for the distance Equation (1.18.1) and Equation (1.18.2) are equivalent.

Hint. Plug rectangular coordinates for the position vectors into Equation (1.18.2) to obtain Equation (1.18.1).

1.19 Scalar Fields

The electrostatic potentials, V, and the gravitational potential, Φ, are examples of scalar fields. A scalar field is any scalar-valued physical quantity (i.e. a number with units attached) at every point in space. It may be useful to think of the temperature in a room, T, as your iconic example of a scalar field.

The symbol $\vec{\boldsymbol{r}}$ represents the position vector which points from an arbitrary fixed origin (that you get to pick once and for all at the beginning of any problem and must use consistently thereafter) to a given point in space. We often write the symbol that represents a scalar field as $V(\vec{\boldsymbol{r}})$ where the position vector ($\vec{\boldsymbol{r}}$) not only reminds us that the scalar field may vary from point to point in space, but also give us a coordinate independent symbol to describe the point at which we are evaluating the field. Similarly, we write $V(\vec{\boldsymbol{r}})$, $\Phi(\vec{\boldsymbol{r}})$, or $T(\vec{\boldsymbol{r}})$ for the electrostatic potential, the gravitational potential, or the temperature, respectively. Even though the symbol $\vec{\boldsymbol{r}}$ contains a vector sign, the name of the scalar field (e.g. V, Φ, or T) does not, since the value of the scalar field at each point is a number, *not* a vector. Several alternative notations are commonly used to denote the point at which the scalar field is being evaluated, for example $V(P)$ (where P is intended to represent the "point" at which the field is evaluated) or $V(x, y, z)$ (where a coordinate system has been chosen).

1.20 Vector Fields

A *vector field*, $\vec{\boldsymbol{F}}$, is a function whose output is a vector at each point in the domain of the function. Each such vector should be thought of as "living" (having its tail at) the point at which it is defined, rather than at the origin. A vector field is often written as any of $\vec{\boldsymbol{F}}(P)$, $\vec{\boldsymbol{F}}(\vec{\boldsymbol{r}})$, $\vec{\boldsymbol{F}}(x,y,z)$, etc., that assigns a vector to each point in the domain, designated by P, $\vec{\boldsymbol{r}}$, or (x,y,z), respectively.

Vector fields can be expanded with respect to any basis, so that we can write

$$\begin{aligned}\vec{\boldsymbol{F}} &= F_x\,\hat{\boldsymbol{x}} + F_y\,\hat{\boldsymbol{y}} + F_z\,\hat{\boldsymbol{z}} && \text{(rectangular)}\\ &= F_s\,\hat{\boldsymbol{s}} + F_\phi\,\hat{\boldsymbol{\phi}} + F_z\,\hat{\boldsymbol{z}} && \text{(cylindrical)}\\ &= F_r\,\hat{\boldsymbol{r}} + F_\theta\,\hat{\boldsymbol{\theta}} + F_\phi\,\hat{\boldsymbol{\phi}} && \text{(spherical)}\end{aligned}$$

where F_x is called the *component of* $\vec{\boldsymbol{F}}$ *with respect to* x, or simply the x-*component* of $\vec{\boldsymbol{F}}$, and similarly for the other components. [1] More information about the curvilinear basis vectors can be found in Section 1.12. Explicit examples are provided by the polar basis vectors $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{\phi}}$, which are shown in Figure 1.20.1. [2]

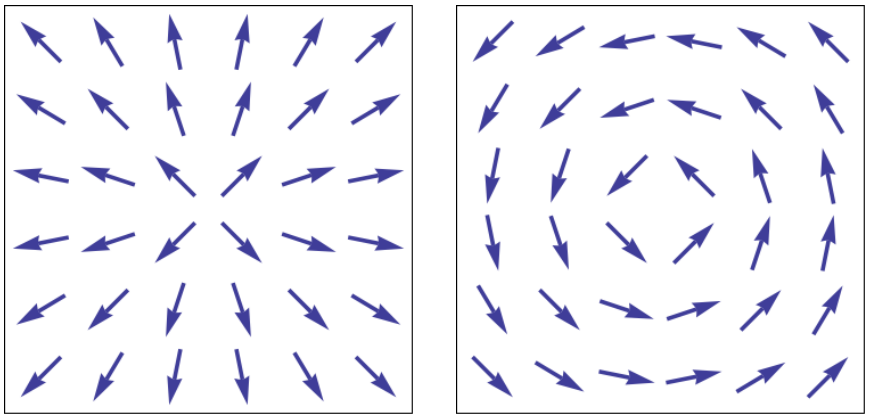


Figure 1.20.1 The polar basis vector fields $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{\phi}}$.

You can generate your own examples by editing the Sage code below.

```
x,y=var('x,y')
p=plot_vector_field((y,x), (x,-10,20), (y,-10,10))
show(p,aspect_ratio=1)
```

1.21 The Cross Product

The cross product is fundamentally a directed area. The *magnitude* of the cross product is defined to be the area of the parallelogram whose sides are the two vectors in the cross product.

[1] Do not confuse the physicists' notation F_x for the x-component of a vector or vector field with the mathematicians' notation f_x for the partial derivative of f with respect to x. The distinction will become obvious from the context as you develop experience.

[2] The software used to create Figure 1.20.1 incorrectly draws each vector *centered* at the point it lives at, rather than putting the *tail* of the vector at this point. Most graphing programs make this mistake; Sage is one of the few exceptions.

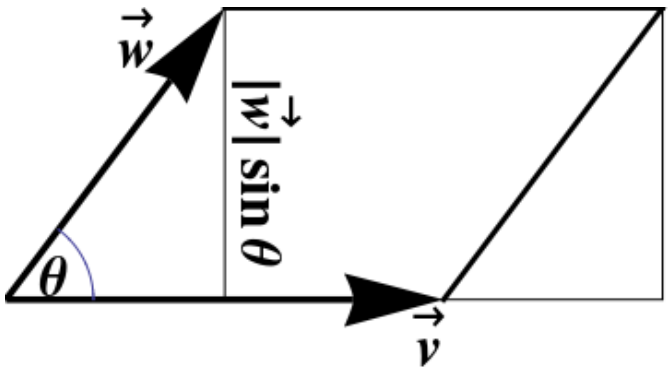


Figure 1.21.1 The cross product as a directed area.

In the figure above, the height of the parallelogram is $|\vec{\boldsymbol{w}}| \sin\theta$, so its area is

$$|\vec{\boldsymbol{v}} \times \vec{\boldsymbol{w}}| = |\vec{\boldsymbol{v}}||\vec{\boldsymbol{w}}| \sin\theta \tag{1.21.1}$$

which is therefore the magnitude of the cross product.

An immediate consequence of Equation (1.21.1) is that, if two vectors are parallel, their cross product is zero,

$$\vec{\boldsymbol{v}} \parallel \vec{\boldsymbol{w}} \iff \vec{\boldsymbol{v}} \times \vec{\boldsymbol{w}} = \vec{\boldsymbol{0}}. \tag{1.21.2}$$

The *direction* of the cross product is given by the right-hand rule: Point the fingers of your right hand along the first vector ($\vec{\boldsymbol{v}}$), and curl your fingers toward the second vector ($\vec{\boldsymbol{w}}$). You may have to flip your hand over to make this work. Now stick out your thumb; that is the direction of $\vec{\boldsymbol{v}} \times \vec{\boldsymbol{w}}$. In the example shown above, $\vec{\boldsymbol{v}} \times \vec{\boldsymbol{w}}$ points out of the page. The right-hand rule implies that

$$\vec{\boldsymbol{w}} \times \vec{\boldsymbol{v}} = -\vec{\boldsymbol{v}} \times \vec{\boldsymbol{w}} \tag{1.21.3}$$

as you should verify for yourself by suitably positioning your hand. Thus, the cross product is not commutative.[1] Another important property of the cross product is that the cross product of a vector with itself is zero,

$$\vec{\boldsymbol{v}} \times \vec{\boldsymbol{v}} = \vec{\boldsymbol{0}} \tag{1.21.4}$$

which follows from any of the preceding three equations.

In terms of the standard orthonormal basis, the geometric formula quickly yields

$$\begin{aligned} \hat{\boldsymbol{x}} \times \hat{\boldsymbol{y}} &= \hat{\boldsymbol{z}}, \\ \hat{\boldsymbol{y}} \times \hat{\boldsymbol{z}} &= \hat{\boldsymbol{x}}, \\ \hat{\boldsymbol{z}} \times \hat{\boldsymbol{x}} &= \hat{\boldsymbol{y}}. \end{aligned}$$

This cyclic nature of the cross product can be emphasized by abbreviating this multiplication table as shown in the figure below. [2]

[1] The cross product also fails to be associative, since for example $\hat{\boldsymbol{x}} \times (\hat{\boldsymbol{x}} \times \hat{\boldsymbol{y}}) = -\hat{\boldsymbol{y}}$ but $(\hat{\boldsymbol{x}} \times \hat{\boldsymbol{x}}) \times \hat{\boldsymbol{y}} = \vec{\boldsymbol{0}}$.

[2] This is really the multiplication table for the unit imaginary quaternions, a number system which generalizes the familiar complex numbers. Quaternions predate vector analysis, which borrowed the i, j, k notation for the rectangular basis vectors, which are often written as $\hat{\boldsymbol{\imath}}$, $\hat{\boldsymbol{\jmath}}$, $\hat{\boldsymbol{k}}$. Here, we have adopted instead the more logical names $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, $\hat{\boldsymbol{z}}$.

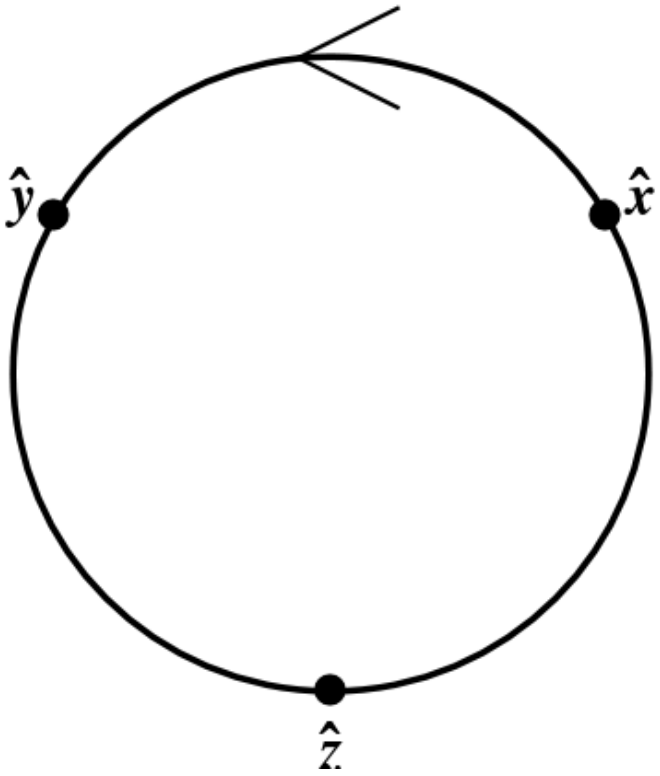


Figure 1.21.2 The cross product multiplication table.

Products in the direction of the arrow get a plus sign; products against the arrow get a minus sign.

Using an orthonormal basis such as $\{\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}\}$, the geometric formula reduces to the standard component form of the cross product. [3] If $\vec{\boldsymbol{v}} = v_x\,\hat{\boldsymbol{x}} + v_y\,\hat{\boldsymbol{y}} + v_z\,\hat{\boldsymbol{z}}$ and $\vec{\boldsymbol{w}} = w_x\,\hat{\boldsymbol{x}} + w_y\,\hat{\boldsymbol{y}} + w_z\,\hat{\boldsymbol{z}}$, then

$$\begin{aligned}\vec{\boldsymbol{v}} \times \vec{\boldsymbol{w}} &= (v_x\,\hat{\boldsymbol{x}} + v_y\,\hat{\boldsymbol{y}} + v_z\,\hat{\boldsymbol{z}}) \times (w_x\,\hat{\boldsymbol{x}} + w_y\,\hat{\boldsymbol{y}} + w_z\,\hat{\boldsymbol{z}}) \\ &= (v_y w_z - v_z w_y)\,\hat{\boldsymbol{x}} + (v_z w_x - v_x w_z)\,\hat{\boldsymbol{y}} + (v_x w_y - v_y w_x)\,\hat{\boldsymbol{z}} \end{aligned} \tag{1.21.5}$$

which is often written as the symbolic determinant

$$\vec{\boldsymbol{v}} \times \vec{\boldsymbol{w}} = \begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ v_x & v_y & v_z \\ w_x & w_y & w_z \end{vmatrix}. \tag{1.21.6}$$

We encourage you to use (1.21.6), rather than simply memorizing (1.21.5). We also encourage you to compute the determinant as described below, rather than using minors; this tends to minimize sign errors. A 3×3 determinant can be computed in the form

[3] This argument uses the distributive property, which must be proved geometrically if one starts with (1.21.1) and the right-hand rule. This is straightforward in two dimensions, but somewhat more difficult in three dimensions. As with the dot product, see our online article.[4]

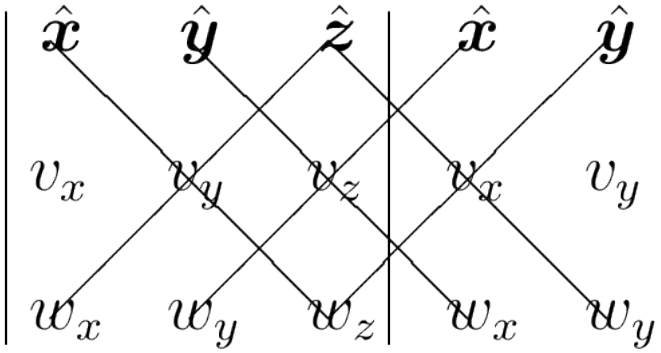


Figure 1.21.3 The determinant.

where one multiplies the terms along each diagonal line, subtracting the products obtained along lines going down to the left from those along lines going down to the right. While this method works only for $(2 \times 2$ and) 3×3 determinants, it emphasizes the cyclic nature of the cross product.

Another important skill is knowing when *not* to use a determinant at all. For simple cross products, such as $(\hat{\boldsymbol{x}} + 3\,\hat{\boldsymbol{y}}) \times \hat{\boldsymbol{z}}$, it is easier to use the multiplication table directly.

It is also worth pointing out that the multiplication table and the determinant method generalize naturally to *any* (right-handed) orthonormal basis; all that is needed is to replace the rectangular basis $\{\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}\}$ by the one being used (in the right order!). For example, in cylindrical coordinates, not only is

$$\hat{\boldsymbol{s}} \times \hat{\boldsymbol{\phi}} = \hat{\boldsymbol{z}} \tag{1.21.7}$$

(and cyclic permutations), but cross products can be computed as

$$\vec{\boldsymbol{v}} \times \vec{\boldsymbol{w}} = \begin{vmatrix} \hat{\boldsymbol{s}} & \hat{\boldsymbol{\phi}} & \hat{\boldsymbol{z}} \\ v_s & v_\phi & v_z \\ w_s & w_\phi & w_z \end{vmatrix} \tag{1.21.8}$$

where of course $\vec{\boldsymbol{v}} = v_s\,\hat{\boldsymbol{s}} + v_\phi\,\hat{\boldsymbol{\phi}} + v_z\,\hat{\boldsymbol{z}}$ and similarly for $\vec{\boldsymbol{w}}$.

A good problem emphasizing the geometry of the cross product is to find the area of the triangle formed by connecting the tips of the vectors $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, $\hat{\boldsymbol{z}}$ (whose base is at the origin).

1.22 Lines and Planes

Two points A and B determine a line. But there are also other ways to describe a line. Rather than specifying *two* points, we can specify just one (A), then give a vector $\vec{\boldsymbol{v}}$ along the line.

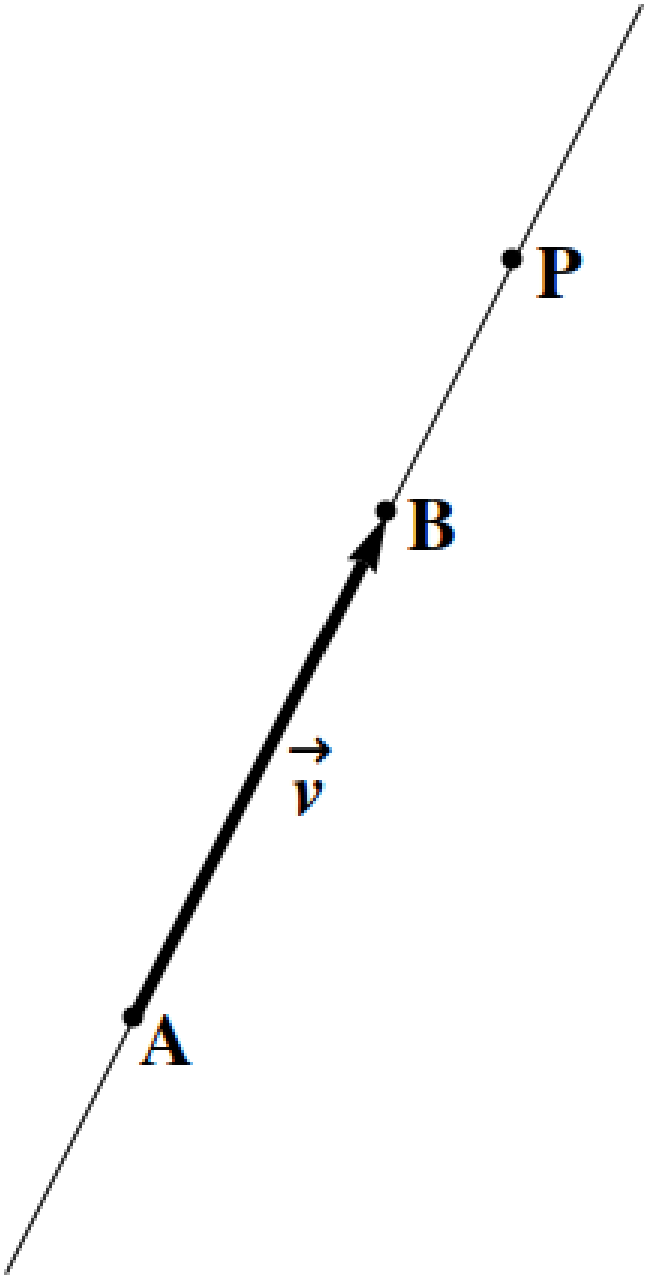


Figure 1.22.1 The geometry behind the vector description of a line.

So let $\vec{\boldsymbol{A}}$ be the vector from the origin to the point A, and $\vec{\boldsymbol{v}}$ be a vector from A that points along the line. Then any other point P on the line can be reached by going to A along $\vec{\boldsymbol{A}}$, then going along $\vec{\boldsymbol{v}}$. Thus, the vector

$$\vec{\boldsymbol{r}}(u) = \vec{\boldsymbol{A}} + \vec{\boldsymbol{v}}\, u \tag{1.22.1}$$

from the origin to P provides a *vector parameterization* of the line. Equivalently, if

$$\vec{\boldsymbol{A}} = a_x\, \hat{\boldsymbol{x}} + a_y\, \hat{\boldsymbol{y}} + a_z\, \hat{\boldsymbol{z}},$$
$$\vec{\boldsymbol{v}} = v_x\, \hat{\boldsymbol{x}} + v_y\, \hat{\boldsymbol{y}} + v_z\, \hat{\boldsymbol{z}},$$

then the line is given by the *parametric equations*

$$x = a_x + v_x\, u,$$
$$y = a_y + v_y\, u,$$
$$z = a_z + v_z\, u,$$

which gives the coordinates (x, y, z) of the point P in terms of the parameter u. A given line can have many parameterizations, depending not only on the choice of the point A on the line and vector $\vec{\boldsymbol{v}}$ along the line, but also on the choice of parameter u.

How do two points determine a line? Using vector addition, you can think of $\vec{\boldsymbol{v}}$ as $\vec{\boldsymbol{B}} - \vec{\boldsymbol{A}}$, and use the vector description above, as shown in Figure 1.22.1.

It takes *three* points A, B, C to determine a plane, but again there are also other descriptions. The orientation of a *line* is given by a vector $\vec{\boldsymbol{v}}$ *along* the line. By contrast, the orientation of a *plane* is given by a vector $\vec{\boldsymbol{w}}$ *perpendicular to* the plane. A plane can therefore be specified by giving a point A and a *normal vector* $\vec{\boldsymbol{w}}$ to the plane at the point A.

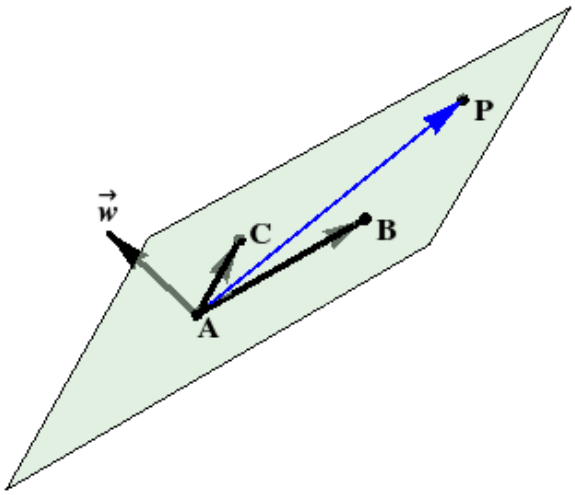


Figure 1.22.2 The geometry behind the vector description of a plane.

If $\vec{\boldsymbol{r}}$ is the vector from the origin to P, then $\vec{\boldsymbol{r}} - \vec{\boldsymbol{A}}$ is a vector in the plane, as shown in Figure 1.22.2. If $\vec{\boldsymbol{w}}$ is perpendicular to the plane, then it must be perpendicular to *any* vector in the plane. In particular, it must be perpendicular to $\vec{\boldsymbol{r}} - \vec{\boldsymbol{A}}$, so that

$$(\vec{\boldsymbol{r}} - \vec{\boldsymbol{A}}) \cdot \vec{\boldsymbol{w}} = 0 \tag{1.22.2}$$

or equivalently

$$\vec{\boldsymbol{r}} \cdot \vec{\boldsymbol{w}} = \vec{\boldsymbol{A}} \cdot \vec{\boldsymbol{w}}. \tag{1.22.3}$$

Inserting the components

$$\vec{\boldsymbol{r}} = x\,\hat{\boldsymbol{x}} + y\,\hat{\boldsymbol{y}} + z\,\hat{\boldsymbol{z}},$$
$$\vec{\boldsymbol{w}} = w_x\,\hat{\boldsymbol{x}} + w_y\,\hat{\boldsymbol{y}} + w_z\,\hat{\boldsymbol{z}},$$

and setting

$$d = \vec{\boldsymbol{A}} \cdot \vec{\boldsymbol{w}} = \text{constant} \tag{1.22.4}$$

leads to

$$w_x x + w_y y + w_z z = d = w_x a_x + w_y a_y + w_z a_z \tag{1.22.5}$$

for the equation of the plane through A with normal direction $\vec{\boldsymbol{w}}$. This equation should look familiar! Note that the constant coefficients of this linear equation are precisely the components of the normal vector!

How do three points determine a plane? Using vector addition, you can construct two vectors in the plane, such as $\vec{\boldsymbol{B}} - \vec{\boldsymbol{A}}$ and $\vec{\boldsymbol{C}} - \vec{\boldsymbol{A}}$. The cross product of these vectors is perpendicular to the plane! Thus, set $\vec{\boldsymbol{w}} = (\vec{\boldsymbol{B}} - \vec{\boldsymbol{A}}) \times (\vec{\boldsymbol{C}} - \vec{\boldsymbol{A}})$, and use the vector description above, as shown in Figure 1.22.2.

1.23 Linearity of the Dot and Cross Products

The linearity of the dot and cross products follows immediately from their algebraic definitions. However, the above derivations of the algebraic formulas from the geometric definitions assumed without comment that both the dot and cross products distribute over addition. To complete the derivation, we must check that linearity follows from the geometric definition. These geometric derivations are shown in Figure 1.23.1 and Figure 1.23.2 below.

For the dot product, we must show that

$$(\vec{\boldsymbol{v}} + \vec{\boldsymbol{u}}) \cdot \vec{\boldsymbol{w}} = \vec{\boldsymbol{v}} \cdot \vec{\boldsymbol{w}} + \vec{\boldsymbol{u}} \cdot \vec{\boldsymbol{w}}$$

which is equivalent to showing that the projection of $\vec{\boldsymbol{v}} + \vec{\boldsymbol{u}}$ along $\vec{\boldsymbol{w}}$ is the sum of the projections of $\vec{\boldsymbol{v}}$ and $\vec{\boldsymbol{u}}$, which is immediately obvious from Figure 1.23.1. In this figure, $\vec{\boldsymbol{v}}$ is shown in blue, $\vec{\boldsymbol{u}}$ in red, their sum in green, and $\vec{\boldsymbol{w}}$ in black.

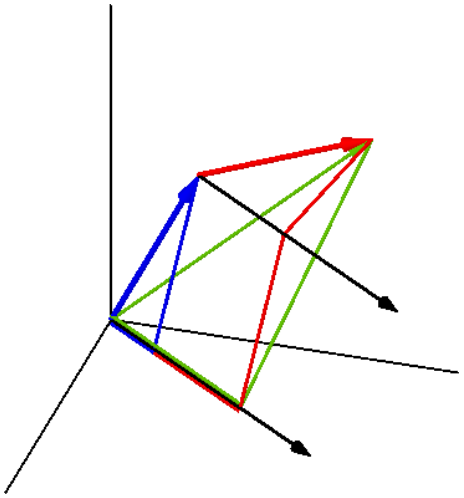


Figure 1.23.1 A geometric proof of the linearity of the dot product.

For the cross product, we must show that

$$\vec{\boldsymbol{w}} \times (\vec{\boldsymbol{v}} + \vec{\boldsymbol{u}}) = \vec{\boldsymbol{w}} \times \vec{\boldsymbol{v}} + \vec{\boldsymbol{w}} \times \vec{\boldsymbol{u}} \tag{1.23.1}$$

which follows with a little thought from Figure 1.23.2, which uses the same color scheme as before.

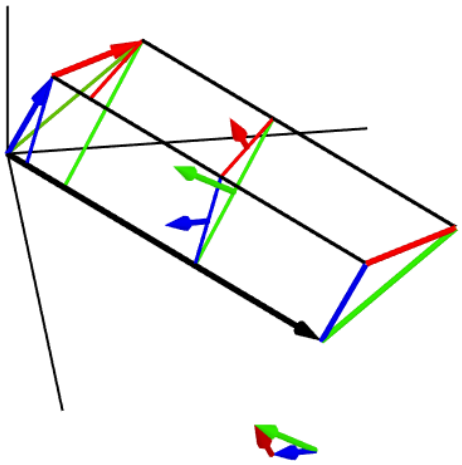


Figure 1.23.2 A geometric proof of the linearity of the cross product.

Consider in turn the vectors $\vec{\boldsymbol{v}}$, $\vec{\boldsymbol{u}}$, and $\vec{\boldsymbol{v}} + \vec{\boldsymbol{u}}$. The cross product of each of these vectors with $\vec{\boldsymbol{w}}$ is proportional to its projection perpendicular to $\vec{\boldsymbol{w}}$. These projections are shown as solid lines in the figure. Since the projections lie in the plane perpendicular to $\vec{\boldsymbol{w}}$, they can be combined into the triangle shown in the middle of the figure. Two of the vectors making up the sides of a triangle add up to the third; in this case, the sides are the projections of $\vec{\boldsymbol{v}}$, $\vec{\boldsymbol{u}}$, and $\vec{\boldsymbol{v}} + \vec{\boldsymbol{u}}$, and the latter is clearly the sum of the first two. But each cross product is now just a rotation of one of the sides of this triangle, rescaled by the length of $\vec{\boldsymbol{w}}$; these are the arrows perpendicular to the faces of the prism. Two of these vectors therefore still add to the third, as indicated by the vector triangle in front of the prism. This establishes (1.23.1).

Chapter 2

Complex Numbers

2.1 The Complex Plane

Complex numbers are a generalization of the real numbers. They are useful in many physics contexts, for example in the study of oscillations and in quantum mechanics. Any calculation you can make with complex numbers, you can make without them, but the calculations will be messier. The time you spend learning how to manipulate complex numbers will pay off many times over.

Definition 2.1.1 Complex Number. A **complex number** z is an ordered pair of real numbers x and y which are distinguished from each other by adjoining the symbol i to the second number:

$$z = x + iy, \tag{2.1.1}$$

together with a multiplication rule described in Section 2.2. ◊

Notation 2.1.1 Real and Imaginary Parts of a Complex Number. The first number, x, is called the **real part** of the complex number z (and denoted $\mathrm{Re}\, z$ or $\Re\, z$) and the second number, y, is called the **imaginary part** of z (and denoted $\mathrm{Im}\, z$ or $\Im\, z$).

Notice that the imaginary part of z is a REAL number.

A number that has zero for its imaginary part is called **real** or, for emphasis, **pure real**. A number that has zero for its real part called **imaginary**, or, for emphasis, **pure imaginary**.

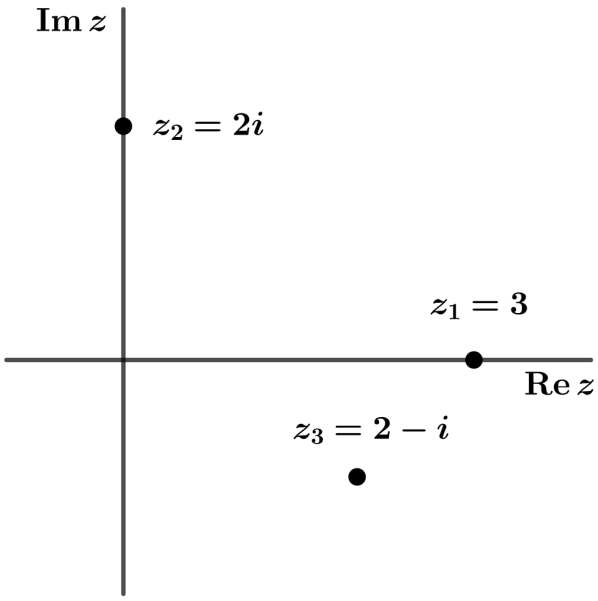


Figure 2.1.2 A pure real number $z_1 = 3$, a pure imaginary number $z_2 = 2i$, and a more generic complex number $z_3 = 2 - i$, plotted as points in the complex plane.

Graphs of Complex Numbers. It is helpful to graph a real number on the real number line. Similarly, it can be helpful to graph a complex number on a 2-d plane where x is recorded on the horizontal axis (called the **real axis**) and y is recorded on the vertical axis (called the **imaginary axis**). This plane, shown in Figure 2.1.2, is called the **complex plane** or, sometimes, an **Argand diagram**.

Analogy with Two-Dimensional Vectors. There is a powerful analogy between vectors in two dimensions and complex numbers that should be obvious from the graph of the complex plane. Every operation that you can do with two dimensional vectors has an analogue with complex numbers. But the reverse is not true; as you will see in Section 2.2, complex numbers have additional structure that comes from a multiplication rule.

2.2 Algebra with Complex Numbers: Rectangular Form

The form of the complex number in Section 2.1:

$$z = x + iy \tag{2.2.1}$$

is called the **rectangular form**, to refer to rectangular coordinates.

We will now extend the definitions of algebraic operations from the real numbers to the complex numbers. For two complex numbers $z_1 = x_1 + iy_1$ and $z_2 = x_2 + iy_2$, we define

Addition and Subtraction. The sum of z_1 and z_2 is given by

$$z_1 + z_2 = (x_1 + iy_1) + (x_2 + iy_2)$$

$$= (x_1 + x_2) + i(y_1 + y_2) \tag{2.2.2}$$

Notice that all we have done is add the real parts of the complex numbers and separately added the imaginary parts. You should be able to convince yourself, with a diagram in the complex plane, that this definition is the same as the parallelogram rule for addition of vectors. The rule for subtraction of complex numbers follows as a straightforward extension.

Multiplication. To define multiplication, we need a new rule, $i^2 = -1$. We say that "i is a square root of minus one". This rule has no analogy for vectors in two dimensions and gives us additional algebraic structure that these vectors do not have.

Now we define multiplication in an obvious way by using the distributive rule of multiplication (i.e. we can "FOIL" everywhere).

$$\begin{aligned} z_1 z_2 &= (x_1 + iy_1)(x_2 + iy_2) \\ &= x_1 y_1 + x_1 i y_2 + i y_1 x_2 + (i)^2 y_1 y_2 \\ &= (x_1 x_2 - y_1 y_2) + i(x_1 y_2 + x_2 y_1) \end{aligned} \tag{2.2.3}$$

It is conventional to rearrange the terms in the product into standard form, i.e. so that the real terms are all together and the pure imaginary terms are all together.

Informal Description of Properties. We see (and/or have assumed) that addition and multiplication of complex numbers is commutative, associative, and distributive. This means that you can do algebra with complex numbers exactly as you are used to; just remember that whenever you see i^2 to replace it with -1.

2.3 Complex Conjugate and Norm

Definition 2.3.1 Complex Conjugate. The **complex conjugate** z^* of a complex number $z = x + iy$ is found by replacing every i by $-i$. Therefore $z^* = x - iy$. (A common alternate notation for z^* is $\bar{z}$.) $\Diamond$

Geometrically, you should be able to see that the complex conjugate of *any* complex number is found by reflecting in the real axis, as shown in Figure 2.3.2.

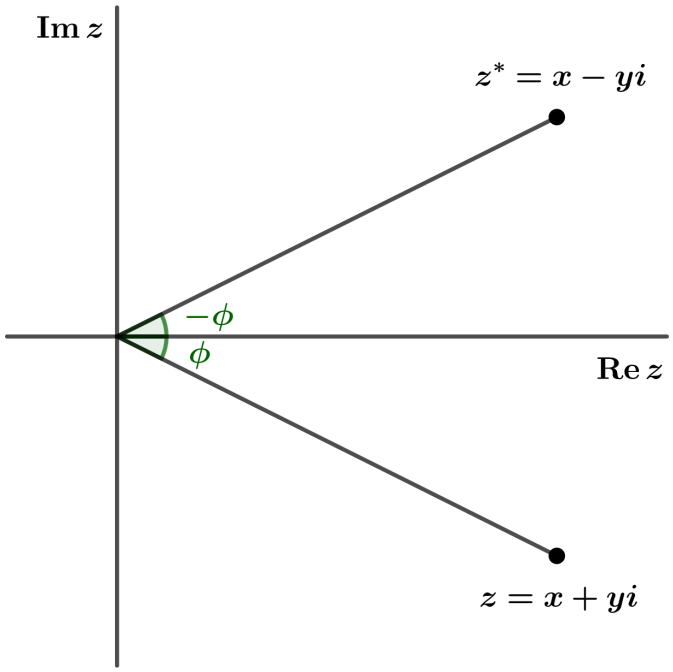


Figure 2.3.2 The point $z = x + iy$ and its complex conjugate $z^* = x - iy$. Note that, in this example, we have deliberately chosen z to be in the fourth quadrant to make you think about which of the variables x, y, and ϕ are positive or negative.

You can find the conjugate of any complicated algebraic expression by taking the conjugate of all of the individual pieces. For example, for a matrix M, the conjugate M^* is found by taking the conjugate of each of the components.

Now let's calculate an important product

$$\begin{aligned} zz^* &= (x + iy)(x - iy) \\ &= x^2 + y^2 \\ &= |z|^2 \end{aligned} \tag{2.3.1}$$

Definition 2.3.3 Norm (or Magnitude) of a Complex Number. Notice that the product zz^* is *always* a positive, real number. The (positive) square root of this number is the distance of the point z from the origin in the complex plane. We call the square root the **norm** or **magnitude** of z and we use the same notation as "absolute value," i.e. $|z|$. In this way, we see that the definition of absolute value, as in $|-2| = 2$, was never "strip off the minus sign," but really "how far is -2 from the origin." ◊

2.4 Division: Rectangular Form

Method for Dividing Two Complex Numbers in Rectangular Form. We can use the concept of complex conjugate to give a strategy for dividing two complex numbers, $z_1 = x_1 + iy_1$ and $z_2 = x_2 + iy_2$. The trick is to multiply by the number 1, in a special form that simplifies the denominator to be a real number and turns division into multiplication.

Consider:

$$\frac{z_1}{z_2} = \frac{z_1}{z_2}\frac{z_2^*}{z_2^*}$$

$$= \frac{z_1 z_2^*}{|z|^2} \tag{2.4.1}$$

The final expression is straightforward to divide into its real and imaginary parts since the denominator is pure real.

In the following activity, you will find the real and imaginary parts of a quotient for the general case. Rather than memorizing the final answer, it will be easier to just repeat this method every time you are dividing two complex numbers.

Activity 2.4.1 Divide Two Complex Numbers in Rectangular Form. Find the real and imaginary components of the complex number $\frac{z_1}{z_2}$ where $z_1 = x_1 + iy_1$ and $z_2 = x_2 + iy_2$.

Solution.

$$\begin{aligned}
\frac{z_1}{z_2} &= \frac{x_1 + iy_1}{x_2 + iy_2} \\
&= \left(\frac{x_1 + iy_1}{x_2 + iy_2}\right)\left(\frac{x_2 - iy_2}{x_2 - iy_2}\right) \\
&= \frac{(x_1 y_1 - x_2 y_2) + i(x_1 y_2 + x_2 y_1)}{x_2^2 + y_2^2} \\
&= \left(\frac{x_1 y_1 - x_2 y_2}{x_2^2 + y_2^2}\right) + i\left(\frac{x_1 y_2 + x_2 y_1}{x_2^2 + y_2^2}\right)
\end{aligned} \tag{2.4.2}$$

2.5 Visualizing Circle Trigonometry

Trigonometry originated as the study of triangles, but a more general definition of the trigonometric functions uses the unit circle.

The projections of P onto the axes determine the signs of $\cos\phi$ and $\sin\phi$ in each quadrant.

For a point P on the unit circle, we *define* $\cos\phi$ as the projection of the point P onto the x-axis and $\sin\phi$ as the projection of the point P onto the y-axis, where ϕ is the usual angle around the origin, measured counterclockwise from the positive x-axis. This construction is shown in Figure 2.5.1.

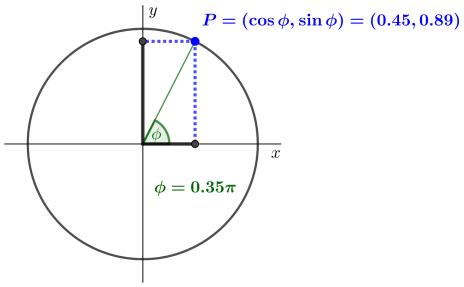


Figure 2.5.1 The coordinates of a point P on the unit circle are $(x, y) = (\cos\phi, \sin\phi)$

Activity 2.5.1 The Relationship between the Unit Circle and Graphs of $\cos\phi$ and $\sin\phi$. To the right of a plot of the unit circle, inspired by Figure 2.5.1, make a plot of $\sin\phi$ vs. ϕ. Align the vertical dimensions and spacing on the two plots so that it's easy to see the relationship. To see a similar relationship for $\cos\phi$, where should you place the plot of $\cos\phi$ vs. ϕ?

Solution. The graphs of $\cos\phi$ vs. ϕ should be turned sideways and placed

below the unit circle, as illustrated in Figure 2.5.2.

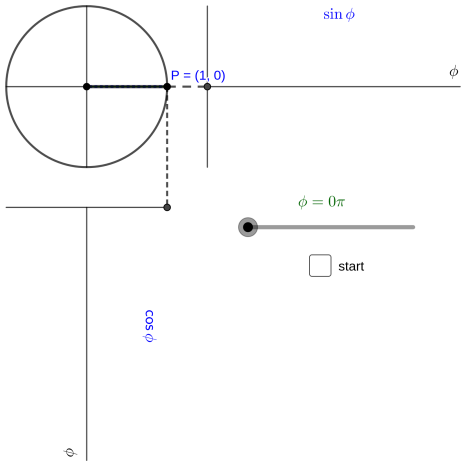


Figure 2.5.2 This combined figure shows the relationship between a point P moving around the unit circle and the (rectangular) graphs of $\cos\phi$ and $\sin\phi$, plotted as functions of ϕ.

2.6 Euler's Formula

As soon as we allow complex numbers into our mathematics, we also need to understand how to extend the definition of familiar functions of real-valued arguments to complex-valued arguments. Most of these extensions are based on Euler's formula.

Definition 2.6.1 Euler's formula.

When evaluated for the special angle $\phi = \pi$, Euler's formula relates the five most important constants in mathematics! $e^{i\pi} + 1 = 0$

The formula

$$e^{i\phi} = \cos\phi + i\sin\phi, \tag{2.6.1}$$

called **Euler's formula**, defines the exponential of a pure imaginary number $i\phi$ in terms of the sine and cosine of a real number ϕ. ◊

Frequently used formulas. We can rearrange Euler's formula and its complex conjugate

$$e^{-i\phi} = \cos\phi - i\sin\phi \tag{2.6.2}$$

to find expressions for $\sin\phi$ and $\cos\phi$ in terms of complex exponentials:

$$\cos\phi = \frac{1}{2}(e^{i\phi} + e^{-i\phi}) \tag{2.6.3}$$

$$\sin\phi = \frac{1}{2i}(e^{i\phi} - e^{-i\phi}). \tag{2.6.4}$$

You will use these expressions for sine and cosine frequently. Make sure you can recognize the right-hand sides of these equations.

Activity 2.6.1 Proofs of Euler's Formula. Euler's formula can be "proved" in two ways:

1. Expand the left-hand and right-hand sides of Euler's formula (2.6.1) in terms of known power series expansions. Compare equal powers.

2. Show that both the left-hand and right-hand sides of Euler's formula

(2.6.1) are solutions of the same second order linear differential equation with constant coefficients. Since only two solutions of a second order linear equation are linearly independent, it must be true that $e^{i\phi}$ is a linear combination of $\cos\phi$ and $\sin\phi$, i.e.

$$e^{i\phi} = A\cos\phi + B\sin\phi. \tag{2.6.5}$$

Choose boundary conditions and known properties of the exponential function to show that $A = 1$ and $B = i$.

Note: If you only know properties of the exponential function for real numbers, then Euler's formula and the "proofs" above are not really proofs, rather they are the definition of the exponential for a pure imaginary argument. Technically, this happens through a process called *analytic continuation*, see Section 2.10.

2.7 Exponential Form

Definition 2.7.1 The Exponential Form of a Complex Number. If we use polar coordinates

$$x = r\cos\phi \tag{2.7.1}$$
$$y = r\sin\phi \tag{2.7.2}$$

to describe the complex number $z = x + iy$, we can factor out the r and use Euler's formula to obtain **the exponential form of the complex number $\boldsymbol{z = re^{i\phi}}$**:

$$\begin{aligned} z &= x + iy \\ &= r\cos\phi + ir\sin\phi \\ &= r(\cos\phi + i\sin\phi) \\ &= re^{i\phi} \end{aligned} \tag{2.7.3}$$

◊

Geometric Interpretation. The parameters r and ϕ inherit their geometric interpretation from polar coordinates, i.e. r represents the distance of z from the origin in the complex plane and ϕ represents the polar angle, measured in radians, counterclockwise from the real axis, as shown in Figure 2.7.2

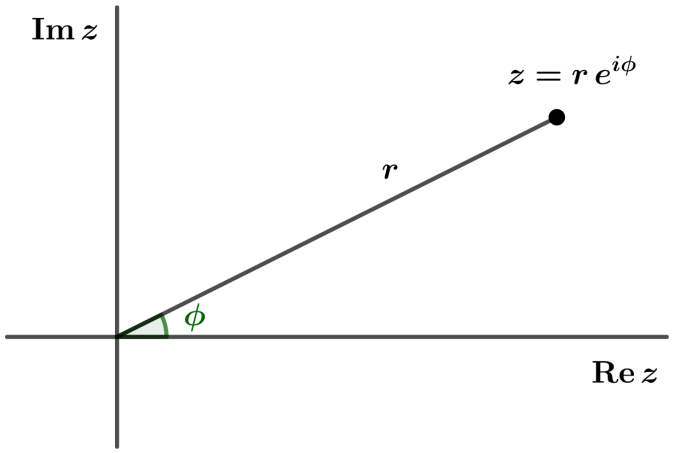


Figure 2.7.2 The point $z = re^{i\phi}$.

2.8 Algebra with Complex Numbers: Exponential Form

The paragraphs below discuss how to do basic arithmetic operations for two complex numbers $z_1 = r_1 e^{i\phi_1}$ and $z_2 = r_2 e^{i\phi_2}$.

Addition and Subtraction. There is nothing simple you can do to simplify the sum and difference of two complex numbers written in exponential form, other than to convert them to rectangular form.

COMING SOON: Factoring out a common phase.

Multiplication and Division. It is easier to do multiplication and division of two complex numbers in exponential form than in rectangular form:

$$\begin{aligned} z_1 z_2 &= r_1 e^{i\phi_1}\, r_2 e^{i\phi_2} \\ &= r_1 r_2 e^{i(\phi_1+\phi_2)} \end{aligned} \tag{2.8.1}$$

$$\begin{aligned} \frac{z_1}{z_2} &= r_1 e^{i\phi_1} / r_2 e^{i\phi_2} \\ &= \frac{r_1}{r_2} e^{i(\phi_1-\phi_2)} \end{aligned} \tag{2.8.2}$$

Notice that the magnitudes of the two complex numbers multiply (or divide) whereas the angles add (or subtract).

2.9 Visualizing the Exponential Function

Using Euler's formula Section 2.6, we now know how to understand the exponential function for both real variables e^x and for pure imaginary variables $e^{iy} = \cos y + i \sin y$. What happens when we put these ideas together? We'd like to extend the definition of the exponential function to be valid when the independent variable is an arbitrary complex number $z = x + iy$. In particular, let's extend the definition so that common exponential rule

$$e^{z_1+z_2} = e^{z_1} e^{z_2} \tag{2.9.1}$$

still holds. (Extending the domain of a function from the reals to the complexes is called analytic continuation, see Section 2.10).

Don't use the exponential form $z = re^{i\phi}$ in this calculation or you will end up having to evaluate exponentials of exponentials

$$e^z = e^{re^{i\phi}}. \tag{2.9.2}$$

Definition 2.9.1 The Exponential of a Complex Number. Using these properties, we see that

$$\begin{aligned} e^z &= e^{x+iy} \\ &= e^x\, e^{iy} \\ &= e^x\,(\cos y + i \sin y) \\ &= e^x \cos y + ie^x \sin y, \end{aligned}$$

The exponential of a complex number is also a complex number; the real and imaginary parts are products of real exponentials and real cosines and sines. ◊

To graph a complex-valued function of a complex variable, we would need to live in four dimensions: two for the input variable (domain) and two for the output variable (range). A common way to handle this problem is to plot the real and imaginary parts of the output on separate graphs, so that, in each case we only need two dimensions for the input variable and one for the output. The following activity explores such graphs for the real part of the exponential function $\operatorname{Re} e^z = e^x \cos y$.

Activity 2.9.1 Visualizing the Exponential Function of a Complex Variable. Look at the figure below. The slider on the left-hand plot chooses various straight-line cross-sections of the complex-plane which range from the positive x-axis when $\theta = 0$ to the negative y-axis when $\theta = -\pi/2$. Start by moving the slider and seeing what happens to the green line segment in the right-hand plot while it is still in its initial position; this shows you the domain.

Next, click and drag on the right-hand plot (up and to the right) to rotate the graph until it looks three-dimensional. Now, on the right-hand graph, you are seeing the full graph of the real part of the exponential function $\operatorname{Re} e^z = e^x \cos y$. Move the slider back and forth between its two limiting cases: the real-valued exponential function e^x when $y = 0$ to the real-valued trigonmetric function $\cos y$ when $x = 0$. The left-hand graph shows just a graph of the cross-section, so its easier to see.

Between the two limiting cases, notice how the cosine function $\cos y$ creates wiggles and the real exponential function e^x makes the magnitude of the wiggles increase for larger values of x.

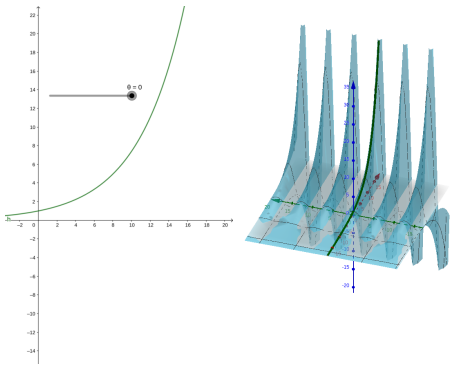


Figure 2.9.2 The graph of $\operatorname{Re} e^z = \operatorname{Re} e^{x+iy} = e^x \cos y$.

2.10 Functions of a Complex Variable

In Section 2.9, we extended the definition of the exponential function to include complex numbers as inputs and in (2.6.3) and (2.6.4) we defined the sine and cosine of a pure imaginary argument. We can go further and extend the sine and cosine functions to be valid for a general complex-valued argument z. We define:

$$\cos z = \frac{1}{2}(e^{iz} + e^{-iz}) \tag{2.10.1}$$

$$\sin z = \frac{1}{2i}(e^{iz} - e^{-iz}) \tag{2.10.2}$$

Definition 2.10.1 Analytic Continuation. The process of extending the definition of a function from a real-valued argument to a complex-valued argument is called **analytic continuation**. ♢

This process is done to make the extension as smooth (i.e. differentiable) as possible. You can learn more about analytic continuation in a course on complex-variable theory. This beautiful mathematics goes well beyond the current scope of this text.

The analytic continuations for powers and roots is discussed in Section 2.11 and for logarithms in Section 2.12

To Remember. The good news is that any formulas that you memorized for real exponentials, real trigonometric functions, powers and roots, and logarithms also apply to their analytic continuations. In particular:

$$e^{z_1+z_2} = e^{z_1}e^{z_2} \tag{2.10.3}$$

Also, the analytic continuations of these common functions of a real variable are unique.

2.11 Powers and Roots of Complex Numbers

If a complex number z is written in exponential form:

$$z = re^{i\phi}, \tag{2.11.1}$$

then the nth power of z is:

$$z^n = r^n\,(e^{i\phi})^n$$

$$= r^n \, e^{in\phi} \tag{2.11.2}$$

and we see that the distance of the point z from the origin in the complex plane has been raised to the nth power, but the angle has been multiplied by n. Similarly, an nth root of z is:

$$z^{\frac{1}{n}} = r^{\frac{1}{n}} e^{i\frac{\phi}{n}}. \tag{2.11.3}$$

For example, a square root of $-4 = 4\exp(i\pi)$ is given by:

$$\begin{aligned} z^{\frac{1}{2}} &= (4e^{i\pi})^{\frac{1}{2}} \\ &= 2e^{\frac{i\pi}{2}} \\ &= 2i \end{aligned} \tag{2.11.4}$$

This is one of the square roots of -4; what about the other root?

It turns out that we can find the other root by including in our original expression for z the multiplicity of angles, all of which give the same point in the complex plane, i.e.

$$z = r \, e^{i\pi + i2\pi m} \tag{2.11.5}$$

where m is any positive or negative integer. Now, when we take the root, we get an infinite number of different factors of the form $\exp(i\frac{2\pi m}{n})$. How many of these correspond to different geometric angles in the complex plane? For $m = \{0, 1, \ldots, n-1\}$, we will get different angles in the complex plane, but as soon as $m = n$ the angles will repeat. Therefore, we find n distinct nth roots of z. If z is real and positive, then one of these roots will be the positive, real nth root that you learned about in high school.

FIXME add an example of cube roots with a picture. Show that the roots are equally spaced around a circle in the complex plane with radius $r^{1/n}$.

2.12 Logarithms of Complex Numbers

How can we extend the logarithm function to complex numbers? We would like to retain the algebraic property that the logarithm of a product is the sum of the logarithms:

$$\ln(ab) = \ln a + \ln b \tag{2.12.1}$$

Then, if we write the complex number z in exponential form:

$$z = r \, e^{i(\phi + 2\pi m)} \tag{2.12.2}$$

and use the property (2.12.1), we find:

$$\begin{aligned} \ln z &= \ln(r \, e^{i(\phi+2\pi m)}) \\ &= \ln r + \ln(e^{i(\phi+2\pi m)}) \\ &= \ln r + i(\phi + 2\pi m) \end{aligned} \tag{2.12.3}$$

The logarithm function (for complex numbers) is an example of a multiple-valued function. All of the multiple-values of the logarithm have the same real part $\ln r$ and the imaginary parts all differ by 2π.

An interesting problem to try is to find $\ln(-1)$. You were probably told in high school algebra that the logarithms of negative numbers do not exist.

Chapter 3

Operations with Matrices

3.1 Matrix Addition

For matrix addition to be defined, both matrices must be of the same dimension, that is, both matrices must have the same number of rows and columns. Addition then proceeds by adding corresponding components, as in

$$C_{ij} = A_{ij} + Bij. \tag{3.1.1}$$

For example, if

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad B = \begin{pmatrix} e & f \\ g & h \end{pmatrix}, \tag{3.1.2}$$

then

$$A + B = \begin{pmatrix} a & b \\ c & d \end{pmatrix} + \begin{pmatrix} e & f \\ g & h \end{pmatrix} = \begin{pmatrix} a+e & b+f \\ c+g & d+h \end{pmatrix}. \tag{3.1.3}$$

Similarly,

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{pmatrix} + \begin{pmatrix} 7 & 8 \\ 9 & 10 \\ 11 & 12 \end{pmatrix} = \begin{pmatrix} 8 & 10 \\ 12 & 14 \\ 16 & 18 \end{pmatrix}. \tag{3.1.4}$$

However,

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} + \begin{pmatrix} 5 & 6 & 7 \\ 8 & 9 & 10 \\ 11 & 12 & 13 \end{pmatrix} \tag{3.1.5}$$

is undefined.

3.2 Scalar Multiplication

A matrix can be multiplied by a scalar, in which case each element of the matrix is multiplied by the scalar. In components,

$$C_{ij} = \lambda A_{ij} \tag{3.2.1}$$

where λ is a scalar, that is, a complex number. For example, if

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{3.2.2}$$

then

$$3A = 3 \cdot \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 3a & 3b \\ 3c & 3d \end{pmatrix}. \tag{3.2.3}$$

Checkpoint 3.2.1 Try it yourself: Scalar Multiplication. Compute:

$$i \cdot \begin{pmatrix} 1 & i \\ -2i & 3 \end{pmatrix}. \tag{3.2.4}$$

Solution.

$$\begin{aligned} i \cdot \begin{pmatrix} 1 & i \\ -2i & 3 \end{pmatrix} &= \begin{pmatrix} (i)(1) & (i)(i) \\ (i)(-2i) & (i)(3) \end{pmatrix} \\ &= \begin{pmatrix} i & -1 \\ 2 & 3i \end{pmatrix}. \end{aligned} \tag{3.2.5}$$

3.3 Matrix Multiplication

Matrices can also be multiplied together, but this operation is somewhat complicated. Watch the progression in the examples below; basically, the elements of the row of the first matrix are multiplied by the corresponding elements of the column of the second matrix. Matrix multiplication can be written in terms of components as

$$C_{ij} = \sum_k A_{ik} B_{kj}. \tag{3.3.1}$$

The simplest example is

$$\begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} e \\ g \end{pmatrix} = ae + bg \tag{3.3.2}$$

which should remind you of the dot product. Somewhat more complicated examples are

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} e \\ g \end{pmatrix} = \begin{pmatrix} ae + bg \\ ce + dg \end{pmatrix} \tag{3.3.3}$$

and

$$\begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} e & f \\ g & h \end{pmatrix} = \begin{pmatrix} ae + bg & af + bh \end{pmatrix}. \tag{3.3.4}$$

A more general example, combining these ideas, is given by

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} e & f \\ g & h \end{pmatrix} = \begin{pmatrix} ae + bg & af + bh \\ ce + dg & cf + dh \end{pmatrix}. \tag{3.3.5}$$

and a numerical example is

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \begin{pmatrix} 5 & 6 \\ 7 & 8 \end{pmatrix} = \begin{pmatrix} 1(5) + 2(7) & 1(6) + 2(8) \\ 3(5) + 4(7) & 3(6) + 4(8) \end{pmatrix} = \begin{pmatrix} 19 & 22 \\ 43 & 50 \end{pmatrix}. \tag{3.3.6}$$

Note however that

$$\begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} c & d \end{pmatrix} \tag{3.3.7}$$

is undefined. For matrix multiplication to be defined, the number of columns of the matrix on the left must equal the number of rows of the matrix on the right.

Checkpoint 3.3.1 Try it yourself: Matrix Multiplication. Compute

$$\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{3.3.8}$$

Solution.

$$\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} (1)(1)+(i)(-1) \\ (-i)(1)+(1)(-1) \end{pmatrix} = \begin{pmatrix} 1-i \\ -1-i \end{pmatrix}.$$

Definition 3.3.2 Outer Product. In the special case of a column times a row, the matrix multiplication is called an **outer product**. ◊

The outer product has an important geometric interpretation, especially when the column and row are Hermitian adjoints of each other, see Section 5.6. For example, the following is an outer product:

$$\begin{pmatrix} a \\ b \end{pmatrix} \begin{pmatrix} a^* & b^* \end{pmatrix} = \begin{pmatrix} aa^* & ab^* \\ ba^* & bb^* \end{pmatrix}. \tag{3.3.9}$$

3.4 Transpose

The transpose of a matrix is obtained by interchanging rows and columns. In terms of components,

$$(A_{ij})^T = A_{ji}. \tag{3.4.1}$$

For example,

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Longrightarrow A^T = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \tag{3.4.2}$$

and

$$B = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \Longrightarrow B^T = \begin{pmatrix} a & d & g \\ b & e & h \\ c & f & i \end{pmatrix}. \tag{3.4.3}$$

A square matrix is called *symmetric* if it is equal to its transpose, that is, if $A = A^T$.

Non-square matrices also have transposes, for example

$$v = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Longrightarrow v^T = \begin{pmatrix} x & y & z \end{pmatrix}. \tag{3.4.4}$$

3.5 Hermitian Adjoint

The Hermitian adjoint of a matrix is the same as its transpose except that along with switching row and column elements you also complex conjugate all the elements. If all the elements of a matrix are real, its Hermitian adjoint and transpose are the same. In terms of components,

$$(A_{ij})^\dagger = A^*_{ji}. \tag{3.5.1}$$

For example, if

$$A = \begin{pmatrix} 1 \\ i \\ -2i \end{pmatrix} \tag{3.5.2}$$

then

$$A^\dagger = \begin{pmatrix} 1 & -i & 2i \end{pmatrix}. \tag{3.5.3}$$

A matrix is called *Hermitian* if it is equal to its adjoint, $A = A^\dagger$.

Checkpoint 3.5.1 Try it yourself: Hermitian Adjoint. Compute $B^\dagger$ if

$$B = \begin{pmatrix} 1 & i \\ -5i & i \end{pmatrix}. \tag{3.5.4}$$

Solution.

$$B^\dagger = (B^T)^* = \begin{pmatrix} 1 & -5i \\ i & i \end{pmatrix}^* = \begin{pmatrix} 1 & 5i \\ -i & -i \end{pmatrix}. \tag{3.5.5}$$

3.6 Dot Products

The geometric, coordinate independent definition of the dot product of two vectors $\vec{v}$ and $\vec{w}$, thought of as arrows in space, is

$$\vec{v} \cdot \vec{w} = |\vec{v}||\vec{w}| \cos\gamma \tag{3.6.1}$$

where γ is the angle between $\vec{v}$ and $\vec{w}$. If we represent the two vectors by their components in a coordinate system

$$\vec{v} \doteq \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} \qquad \vec{w} \doteq \begin{pmatrix} w_x \\ w_y \\ w_z \end{pmatrix} \tag{3.6.2}$$

then the geometric definition is equivalent

We are not proving the equivalence here. Please see our online paper with cool, rotatable figures!! ***Update the figures and add a link here.***

to the algebraic definition

$$\vec{v} \cdot \vec{w} = \begin{pmatrix} v_x & v_y & v_z \end{pmatrix} \begin{pmatrix} w_x \\ w_y \\ w_z \end{pmatrix} \tag{3.6.3}$$

$$= v_x w_x + v_y w_y + v_z w_z \tag{3.6.4}$$

In physics, the dot product is most often used for two purposes: to find the length of a vector $|\vec{v}| = \sqrt{\vec{v} \cdot \vec{v}}$ and to show that two vectors are perpendicular to each other $\vec{v} \perp \vec{w} \Leftrightarrow \vec{v} \cdot \vec{w} = 0$.

Activity 3.6.1 Show, from the geometric definition of the dot product (3.6.1), that the length of a vector is given by $|\vec{v}| = \sqrt{\vec{v} \cdot \vec{v}}$. Repeat for the algebraic definition (3.6.4).

Activity 3.6.2 Show, from the geometric definition of the dot product (3.6.1), that the two vectors are perpendicular if and only if their dot product is zero $\vec{v} \perp \vec{w} \Leftrightarrow \vec{v} \cdot \vec{w} = 0$. Repeat for the algebraic definition (3.6.4).

The generalization of the dot product to vectors with complex components can be found in Section 3.7.

3.7 Inner Products for Complex Vectors

Column matrices play a special role in physics, where they are interpreted as *vectors* or, in quantum mechanics, *states*. To remind us of this uniqueness they have their own special notation; introduced by Dirac, called *bra-ket* notation. In bra-ket notation, a column matrix, called a *ket*, can be written

$$|v\rangle \doteq \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}. \tag{3.7.1}$$

The Hermitian adjoint of this vector is called a *bra*

$$\langle v| \doteq (|v\rangle)^\dagger = \begin{pmatrix} v_x^* & v_y^* & v_z^* \end{pmatrix}. \tag{3.7.2}$$

Notice that we are *not* assuming that the components of the vector are real.

Now we want to generalize the concept of dot product from Section 3.6 to this case where the components of the vector or state are not necessarily real. This generalization is technically called an *inner product* although many scientists will still casually use the term dot product. If we take $|v\rangle$ to be a 3-vector with components v_x, v_y, v_z as above, then the inner product of this vector with itself is called a *braket*

$$\langle v|v\rangle = \begin{pmatrix} v_x^* & v_y^* & v_z^* \end{pmatrix} \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = |v_x|^2 + |v_y|^2 + |v_z|^2 \tag{3.7.3}$$

which is a positive real number. We will call the square root of this positive real number the magnitude (or, more casually, the length) of the vector, even when the vector is abstract and there is no length that we would be able to measure with a ruler. Similarly, we will say that two vectors are orthogonal (or, more casually, perpendicular) whenever their inner product is zero, even if there is no angle that we could measure with a protractor.

In physics, you will encounter many other abstract spaces that have the same algebraic properties as vectors and dot products. A list of these abstract properties and some examples can be found in Section 14.1 and Section 14.2.

3.8 Trace

The trace of a (square) matrix is just the sum of all of its diagonal elements. In terms of components,

$$\mathrm{tr}(A) = \sum_i A_{ii}. \tag{3.8.1}$$

For example, if

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix} \tag{3.8.2}$$

then

$$\mathrm{tr}(A) = 1 + 5 + 9 = 15. \tag{3.8.3}$$

Checkpoint 3.8.1 Try it yourself: Trace. Compute $\mathrm{tr}(B)$ if

$$B = \begin{pmatrix} 1 & 34 & 5 \\ 23 & 5 & 98 \\ 132 & 7 & 9 \end{pmatrix}. \tag{3.8.4}$$

Solution.

$$tr(B) = 1 + 5 + 9 = 15. \tag{3.8.5}$$

3.9 Determinants

The determinant of a (square) matrix is somewhat complicated in general, so you may want to check a reference book. The 2×2 and 3×3 cases can be memorized using the examples below.

The determinant of a 2×2 matrix is given by

$$\det \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc. \tag{3.9.1}$$

Notice in the equation above the two common notations for determinant.

The determinant of a 3×3 matrix is computed as follows:

$$\begin{aligned} \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} &= \det \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \\ &= a \cdot \begin{vmatrix} e & f \\ h & i \end{vmatrix} - b \cdot \begin{vmatrix} d & f \\ g & i \end{vmatrix} + c \cdot \begin{vmatrix} d & e \\ g & h \end{vmatrix} \\ &= a \cdot (ei - hf) - b \cdot (di - gf) + c \cdot (dh - ge) \\ &= aei - ahf - bdi + bgf + cdh - cge. \end{aligned} \tag{3.9.2}$$

The smaller 2×2 determinants are called the *cofactors* of the elements a, b, and c, respectively. The minus sign in front of b is part of the cofactor. Cofactors are formed by keeping only what is left after eliminating everything from the row and column where the element desired resides. So, for a, the row elements, b and c, and the column elements, d and g, are eliminated, leaving the 2×2 matrix shown above.

Computing 4×4 matrices is a straightforward extension of the above procedure, but it is easier to just go to a computer!!!

Checkpoint 3.9.1 Try it yourself: Determinant. Compute $\det(B)$ if

$$B = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}. \tag{3.9.3}$$

Solution. The method above extends naturally to square matrices of any size, but there is an easier way to find the determinant of a 3×3 matrix that uses cyclic symmetry. Multiply the numbers on each "forward" diagonal (wrapping around as needed) and add them together, then do the same on each "backward" diagonal, but *subtract* the latter subtotal from the former.

Applying this method to B, we have

$$\begin{aligned} \det(B) = (1)(5)(9) + (2)(6)(7) + (3)(4)(8) \\ - (3)(5)(7) - (1)(6)(8) - (2)(4)(9) = 0 \end{aligned} \tag{3.9.4}$$

You can use the Sage code below to compute the determinant of any matrix.

```
B=matrix([[1,2,3],[4,5,6],[7,8,9]])
det(B)
```

3.10 Inverses

The matrix inverse of a matrix A, denoted A^{-1}, is the matrix such that when multiplied by the matrix A the result is the *identity matrix*. (The identity matrix is the matrix with ones down the diagonal and zeroes everywhere else.)

For 2×2 matrices, if

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \tag{3.10.1}$$

then

$$A^{-1} = \frac{1}{\det(A)} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}. \tag{3.10.2}$$

For 3×3 matrices B, B^{-1} is the transpose of the matrix made of all cofactors of B, divided by the determinant of B. This is easier said in symbols, so if

$$B = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \tag{3.10.3}$$

then

$$B^{-1} = \frac{1}{\det(B)} \begin{pmatrix} \begin{vmatrix} e & f \\ h & i \end{vmatrix} & -\begin{vmatrix} b & c \\ h & i \end{vmatrix} & \begin{vmatrix} b & c \\ e & f \end{vmatrix} \\ -\begin{vmatrix} d & f \\ g & i \end{vmatrix} & \begin{vmatrix} a & c \\ g & i \end{vmatrix} & -\begin{vmatrix} a & c \\ d & f \end{vmatrix} \\ \begin{vmatrix} d & e \\ g & h \end{vmatrix} & -\begin{vmatrix} a & b \\ g & h \end{vmatrix} & \begin{vmatrix} a & b \\ d & e \end{vmatrix} \end{pmatrix} \tag{3.10.4}$$

In both cases, the inverse only exists if the determinant is nonzero.

Checkpoint 3.10.1 Try it yourself: Inverse. Suppose that

$$Q = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}. \tag{3.10.5}$$

What is Q^{-1}? Verify that QQ^{-1} is the identity matrix.

Solution. Using (3.10.2), we have $\det(Q) = (1)(4) - (2)(3) = -2$, so

$$Q^{-1} = -\frac{1}{2}\begin{pmatrix} 4 & -2 \\ -3 & 1 \end{pmatrix} = \begin{pmatrix} -2 & 1 \\ \frac{3}{2} & -\frac{1}{2} \end{pmatrix} \tag{3.10.6}$$

so that

$$\begin{aligned} QQ^{-1} &= \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}\begin{pmatrix} -2 & 1 \\ \frac{3}{2} & -\frac{1}{2} \end{pmatrix} \\ &= \begin{pmatrix} (1)(-2)+(2)(\frac{3}{2}) & (1)(1)+(2)(-\frac{1}{2}) \\ (3)(-2)+(4)(\frac{3}{2}) & (3)(1)+(4)(-\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned} \tag{3.10.7}$$

Chapter 4

Eigenvectors and Eigenvalues

This chapter describes the procedure for finding eigenvectors and eigenvalues. We use *bra-ket* notation. If this notation is unfamiliar, please see a brief explanation in Section 3.7

4.1 What are Eigenvectors?

Eigenvectors appear ubiquitously in physics. For example, they are the fundamental mathematical objects underlying the study of normal modes in classical oscillating systems and the building blocks of states in a quantum theory.

Definition 4.1.1 Eigenvalue/Eigenvector Equation. For a given square matrix A, the **eigenvalue/eigenvector equation** is

$$A|v\rangle = \lambda|v\rangle \tag{4.1.1}$$

A solution $|v\rangle$ of this equation is called an **eigenvector** and the scalar λ is called the **eigenvalue**. ♢

The terms **eigenvector**, **eigenfunction**, and **eigenstate** all refer to equivalent mathematical concepts. (The first is generic, whereas the second is often used in contexts involving differential operators and functions, and the last in quantum mechanics contexts.) The term **eigenvalue**, however, is a different kind of mathematical object. It refers always to the scalar λ.

Notice that the matrix A and the scalar λ are very different mathematical objects. When a *real* matrix acts on an arbitrary *real* vector it can change its length and/or its direction. Eigenvectors are special; the eigenvalue equation says that only their length and not their direction changes. If the matrix is not real, then we lose this clear geometric interpretation, but the same general idea still holds. The eigenvector/eigenvalue equation says that, for the very special vectors, called eigenvectors, when the matrix operates on them they only change by being multiplied by a scalar. Depending on the context, this scalar may be any real number including zero or negative or even a complex number. In some contexts, it may have physical dimensions, such as factors of $\hbar$. Even in these cases, we will still use the language of *length* and *direction*.

In this section, we have introduced the concept of eigenvectors for matrices, but the generalizations to any linear operator see Section 14.8 such as differential operators and eigenfunctions or to abstract Hermitian operators and eigenstates are straightforward.

4.2 Finding Eigenvalues

Informal definition: An eigenvector is a vector whose length may be changed by a transformation, but not its direction .

Method for Finding Eigenvalues of a Square Matrix. In order to find the eigenvalues of a square matrix A, we must find the values of λ such that the equation

$$A|v\rangle = \lambda|v\rangle \tag{4.2.1}$$

admits solutions $|v\rangle$. (The solutions $|v\rangle$ are eigenvectors of A, as discussed in the next section.) Rearranging terms, $|v\rangle$ must satisfy

$$(\lambda I - A)|v\rangle = 0 \tag{4.2.2}$$

where I denotes the identity matrix (of the same size as A). Suppose that the inverse matrix $(\lambda I - A)^{-1}$ exists. Multiplying both sides of (4.2.2) by this inverse would then yield

$$(\lambda I - A)^{-1}(\lambda I - A)|v\rangle = |v\rangle = 0 \tag{4.2.3}$$

which is not a very interesting solution. So, instead, we want $(\lambda I - A)$ *not* to have an inverse. When does this happen?

Claim: *A square matrix A does not have an inverse if and only if* $\det A = 0$.

Theorem 4.2.1 The Eigenvalues of a Square Matrix A. *Thus, the eigenvalues of A are the solutions of the equation* $\det(\lambda I - A) = 0$.

This is one of those cases where the mathematicians can give special cases where some expected eigenvalues are missing, but for undergraduate physics contexts like Hermitian and unitary matrices you will always get n eigenvalues, see Section 5.3 and Section 5.5.

Usually*, this computation yields a polynomial equation in λ, which is of order n if A is an $n \times n$ matrix. Thus, we expect n (complex) eigenvalues, which however might not be distinct.*

Definition 4.2.2 Degeneracy/Multiplicity. In the case of an eigenvalue that is repeated m times, we call the eigenvalue ***m*-fold degenerate**, or, equivalently, **of multiplicity *m***. For more information about degenerate eigenvalues, see Section 4.6. ♢

Example. Suppose $A = \begin{pmatrix} 1 & 2 \\ 9 & 4 \end{pmatrix}$. Then we must solve

$$0 = |\lambda I - A| = \begin{vmatrix} 1 & 2 \\ 9 & 4 \end{vmatrix} = (\lambda - 1)(\lambda - 4) - 18 \tag{4.2.4}$$

or equivalently

$$0 = \lambda^2 - 5\lambda - 14 = (\lambda - 7)(\lambda + 2), \tag{4.2.5}$$

and the eigenvalues in this case are $\lambda = 7$ and $\lambda = -2$.

4.3 Finding Eigenvectors

Examples. Having found the eigenvalues of the example matrix $A = \begin{pmatrix} 1 & 2 \\ 9 & 4 \end{pmatrix}$ in (4.2.2) to be 7 and -2, we can now ask what the corresponding eigenvectors are. We must therefore solve the equation

$$A|v\rangle = \lambda|v\rangle \tag{4.3.1}$$

in the two cases $\lambda = 7$ and $\lambda = -2$. In the first case, we have

$$\begin{pmatrix} 1 & 2 \\ 9 & 4 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 7 \begin{pmatrix} x \\ y \end{pmatrix} \tag{4.3.2}$$

or equivalently

$$\begin{pmatrix} x + 2y \\ 9x + 4y \end{pmatrix} = \begin{pmatrix} 7x \\ 7y \end{pmatrix}. \tag{4.3.3}$$

Thus, we must solve this system of two equations. But we quickly discover that these equations are reduntant, since the first implies $2y = 6x$, while the second implies $3y = 9x$, which is the same condition. This is a good thing! (Why?)

We conclude that *any* vector $\begin{pmatrix} x \\ y \end{pmatrix}$ with $y = 3x$ is an eigenvector of A with eigenvalue 7. To check an explicit example, choose *any* value for x, such as $x = 1$, yielding the vector

$$|v_7\rangle \doteq \begin{pmatrix} 1 \\ 3 \end{pmatrix} \tag{4.3.4}$$

and check by explicit computation that $A\,|v_7\rangle = 7\,|v_7\rangle$, as expected.

Turning to the case $\lambda = -2$, a similar construction yields

$$\begin{pmatrix} 1 & 2 \\ 9 & 4 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = -2 \begin{pmatrix} x \\ y \end{pmatrix} \tag{4.3.5}$$

or equivalently

$$\begin{pmatrix} x + 2y \\ 9x + 4y \end{pmatrix} = \begin{pmatrix} -2x \\ -2y \end{pmatrix}, \tag{4.3.6}$$

and the first equation now yields $2y = -3x$, while the second yields $6y = -9x$. Again, these two equations are redundant; the eigenvectors with eigenvalue -2 satisfy $y = -\frac{3}{2}$. An explicit example is

$$|v_{-2}\rangle \doteq \begin{pmatrix} 2 \\ -3 \end{pmatrix} \tag{4.3.7}$$

and you should again check by explicit computation that $A\,|v_{-2}\rangle = -2\,|v_{-2}\rangle$.

To Remember. The set of equations that you solve for the eigenvectors will always be redundant (or trivial). So you will always have to *choose* one of the components. This freedom leads to the useful property that multiples of eigenvectors are still eigenvectors, see Section 4.4.

4.4 Normalization of Eigenvectors

In Section 3.7, we defined the inner product operation on abstract vectors with complex components, such as

$$|v\rangle \doteq \begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}. \tag{4.4.1}$$

If we take the inner product of this vector with itself,

$$\langle v|v\rangle = \begin{pmatrix} a^* & b^* & \dots \end{pmatrix} \begin{pmatrix} a \\ b \\ \vdots \end{pmatrix}$$

$$= |a|^2 + |b|^2 + \ldots, \tag{4.4.2}$$

the operation always yields a positive, real number. Thus, we can use the square root of this operation $||v\rangle|$.

$$||v\rangle| = \{\langle v|v\rangle\}^{\frac{1}{2}} \tag{4.4.3}$$

to define the **norm** (also called **magnitude** or **length**) of the vector. This definition is a natural generalization of the dot product, see Section 1.8, of a real vector with itself.

Definition 4.4.1 Normalized Vector. From the eigenvalue/eigenvector equation (4.1.1):

$$A\,|v\rangle = \lambda\,|v\rangle \tag{4.4.4}$$

it is straightforward to show that if $|v\rangle$ is an eigenvector of A, then, any multiple $N|v\rangle$ of $|v\rangle$ is also an eigenvector since N can pull through to the left on both sides of the equation.

If a choice of N normalizes a particular vector, then so does any arbitrary complex phase times the original number $Ne^{i\alpha}$ (for α real). Usually, we choose N to be real, for simplicity.

It is always possible to choose the number N to rescale the eigenvector to have length 1. Such an eigenvector is called **normalized**. ◊

4.5 Special Case: Diagonal Matrices

Definition 4.5.1 Diagonal Matrix. A square matrix whose only nonzero entries lie on the main diagonal is called a **diagonal matrix**. ◊

The simplest example of a diagonal matrix is the identity matrix

$$I = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{pmatrix}. \tag{4.5.1}$$

Eigenvalues and Eigenvectors of Diagonal Matrices. It is easy to find the eigenvalues and eigenvectors of a diagonal matrix! For example, consider the matrix

$$A = \begin{pmatrix} \mu & 0 & 0 \\ 0 & \nu & 0 \\ 0 & 0 & \sigma \end{pmatrix}. \tag{4.5.2}$$

The eigenvalues of A are clearly $\{\mu, \nu, \sigma\}$ since

$$\begin{aligned} \det(\lambda I - A) &= \begin{vmatrix} \lambda-\mu & 0 & 0 \\ 0 & \lambda-\nu & 0 \\ 0 & 0 & \lambda-\sigma \end{vmatrix} \\ &= (\lambda-\mu)(\lambda-\nu)(\lambda-\sigma). \end{aligned} \tag{4.5.3}$$

It is much easier to *check* that something is an eigenvector than to find the eigenvectors using the procedure in Section 4.3.

Check that the corresponding eigenvectors are just the **standard basis**

$$\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}. \tag{4.5.4}$$

To Remember. The eigenvalues of a diagonal matrix are just the diagonal elements themselves. The eigenvectors of a diagonal matrix are just the standard basis.

4.6 Degeneracy and Eigenspaces

An Example of Degenerate Eigenvalues. It is not always the case that an $n \times n$ matrix has n *distinct* eigenvectors. In Section 4.2, we defined a repeated eigenvalue to be **degenerate**. For example, consider the matrix

$$B = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix}, \tag{4.6.1}$$

whose eigenvectors are clearly the standard basis. But what are the eigenvalues of B? Again, the answer is obvious: 3 and 5. In such cases, the eigenvalue 3 is a *degenerate* eigenvalue of B, since there are two linearly independent eigenvectors of B with eigenvalue 3. In this case, one also says that 3 is **a repeated eigenvalue of multiplicity 2**.

However, that's not the whole story. Setting

$$|v\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |w\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \tag{4.6.2}$$

we of course have

$$B|v\rangle = 3|v\rangle, \qquad B|w\rangle = 3|w\rangle. \tag{4.6.3}$$

But, by the linearity of matrix operations (see Section 3.2 and Section 3.1), we also have

$$B(a|v\rangle + b|w\rangle) = a\,B|v\rangle + b\,B|w\rangle = 3(a|v\rangle + b|w\rangle), \tag{4.6.4}$$

so that *any* linear combination of $|v\rangle$ and $|w\rangle$ is also an eigenvector of B with eigenvalue 3.

Definition 4.6.1 Eigenspace. An **eigenspace** is the set of all vectors with the same eigenvalue. ◊

The *eigenspace* of B corresponding to eigenvalue 3 is therefore a 2-dimensional vector space (a plane), rather than the 1-dimensional eigenspaces (lines) that occur when the eigenvalues are distinct.

Chapter 5

Special Matrices

5.1 Commuting Matrices

Commuting operators play a very special role in the theory of quantum mechanics.

Definition 5.1.1 Commutator. The **commutator** of two matrices (or operators) is defined by the combination

$$[M, N] \equiv MN - NM. \tag{5.1.1}$$

When acting on a vector, the commutator tells you about the difference between operating in one order and operating in the other order. If the order doesn't matter, then the commutator is zero, $[M, N] = 0$, and the operators M and N are said to **commute**. ♢

Commuting operators have the same (non-degenerate) eigenvectors. Suppose two operators M and N commute, $[M, N] \equiv MN - NM = 0$. Then if M has an eigenvector $|v\rangle$ with *non-degenerate* eigenvalue λ_v, we will show that $|v\rangle$ is also an eigenvector of N.

$$M|v\rangle = \lambda_v|v\rangle \tag{5.1.2}$$

$$N\left(M|v\rangle\right) = M\left(N|v\rangle\right) = \lambda_v\left(N|v\rangle\right) \tag{5.1.3}$$

The last equality shows that $N|v\rangle$ is also an eigenvector of M with the same non-degenerate eigenvalue λ_v. But if this is true, then $N|v\rangle$ must be proportional to $|v\rangle$, i.e.

$$N|v\rangle = \alpha|v\rangle \tag{5.1.4}$$

which is just the statement that $|v\rangle$ is also an eigenvector of N with eigenvalue α.

Note that if λ_v were a degenerate eigenvalue, then we would not have been able to assume that $N|v\rangle$ is proportional to $|v\rangle$.

5.2 Definition of Hermitian Matrices

Definition 5.2.1 Hermitian Matrices. On an $n \times m$ matrix, N, you can take the **Hermitian adjoint** (usually denoted with a dagger, †) which means take both the (complex) conjugate Section 2.3 and the transpose Section 3.4, in either order

$$N^\dagger = N^{*T}. \tag{5.2.1}$$

Two uses of the word "Hermitian". You should not confuse the two uses of the word **Hermitian**. One describes an operation that you can do to matrices–to take the **Hermitian adjoint** (an action), the other describes a matrix with a particular form–a **Hermitian matrix** (an object).

An $n \times n$ (square) matrix M is **Hermitian** if it equals its conjugate transpose, that is, if

$$M^\dagger = M. \tag{5.2.2}$$

If a matrix M is both Hermitian and real, then M is called a **symmetric matrix**. An **anti-Hermitian** matrix is one for which the Hermitian adjoint is the negative of the matrix:

$$M^\dagger = -M. \tag{5.2.3}$$

A matrix which is both anti-Hermitian and real is called **antisymmetric**. ◊

Identifying Hermitian Matrices. For example, let M be a 2×2 complex matrix, so that

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{5.2.4}$$

with $a, b, c, d \in \mathbb{C}$, and its Hermitian adjoint is

$$M^\dagger = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}, \tag{5.2.5}$$

If M is Hermitian, then $M^\dagger = M$, so, we must have

$$a^* = a, b^* = c, d^* = d, \tag{5.2.6}$$

i.e. a and d are real and c is the complex conjugate of b.

In index notation, if the components of M are denoted m_{ij}, then M is Hermitian if and only if

$$m_{ij} = m^*_{ji} \tag{5.2.7}$$

for all i, j. (See also, Section 3.5.) Thus, the diagonal elements of a Hermitian matrix must be real, and the off-diagonal elements come in complex conjugate pairs, paired symmetrically across the main diagonal.

An Important Special Case of Hermitian Matrices. An important special case of a Hermitian matrix can be constructed from any column vector v by computing its outer square, which in traditional vector notation would be written $vv^\dagger$ and in bra/ket notation would be written $|v\rangle\langle v|$. (See Section 5.6 for a description of how such operators are used to produce projections.)

5.3 Properties of Hermitian Matrices

The eigenvalues and eigenvectors of Hermitian matrices Section 5.2 have some special properties.

The eigenvalues of a Hermitian matrix must be real. To see why this relationship holds, start with the eigenvector equation

$$M|v\rangle = \lambda|v\rangle \tag{5.3.1}$$

and multiply on the left by $\langle v|$ (that is, by $v^\dagger$):

$$\langle v|M|v\rangle = \langle v|\lambda|v\rangle = \lambda\langle v|v\rangle. \tag{5.3.2}$$

But we can also compute the Hermitian conjugate (that is, the conjugate transpose) of (5.3.1), which is

$$\langle v|M^\dagger = \langle v|\lambda^*. \tag{5.3.3}$$

Using the fact that $M^\dagger = M$, and multiplying by $|v\rangle$ on the right now yields

$$\langle v|M|v\rangle = \langle v|\lambda^*|v\rangle = \lambda^*\langle v|v\rangle. \tag{5.3.4}$$

Comparing (5.3.2) with (5.3.4) now shows that

$$\lambda^* = \lambda \tag{5.3.5}$$

as claimed.

Eigenvectors corresponding to different eigenvalues must be orthogonal. The argument establishing this relationship is similar to the one above. Suppose that

$$M|v\rangle = \lambda|v\rangle, \tag{5.3.6}$$
$$M|w\rangle = \mu|w\rangle. \tag{5.3.7}$$

Then

$$\langle v|\lambda|w\rangle = \langle v|M|w\rangle = \langle v|\mu|w\rangle \tag{5.3.8}$$

or equivalently

$$(\lambda - \mu)\langle v|w\rangle = 0. \tag{5.3.9}$$

Thus, if $\lambda \neq \mu$, $|v\rangle$ must be orthogonal to $|w\rangle$.

Repeated Eigenvalues. In the case of repeated eigenvalues, it is possible to make a basis orthogonal using a process called **Gram-Schmidt orthogonalization**. (This amounts to simply subtracting off the parts of a given basis that are not orthogonal.)

To Remember. It is always possible to find an orthonormal basis of eigenvectors for any Hermitian matrix.

Sensemaking 5.3.1 Properties of Anti-Hermitian Matrices. Repeat the two proofs above to find similar properties for anti-Hermitian matrices.

Hint 1. Don't forget to use $M^\dagger = -M$.

Hint 2. Don't forget to complex conjugate the eigenvalue, where necessary.

Answer. The eigenvalues are pure imaginary. The eigenvectors corresponding to different eigenvalues are orthogonal.

5.4 Unitary Matrices

An $n \times n$ matrix U is **unitary** if its Hermitian adjoint (i.e. conjugate transpose) is equal to its inverse, that is, if

$$U^\dagger = U^{-1}, \tag{5.4.1}$$

in which case,

$$U^\dagger U = I = UU^\dagger. \tag{5.4.2}$$

If U is both unitary and real, then U is called an **orthogonal** matrix.

Working out the condition for unitarity, it is easy to see that the rows (and similarly the columns) of a unitary matrix U form a (complex) orthonormal basis. Using bra/ket notation, and writing $|v_i\rangle$ for the columns of U, then

$$\langle v_i|v_j\rangle = \delta_{ij}. \tag{5.4.3}$$

We will use unitary matrices in four ways:

1. Unitary matrices preserve the norm of vectors, Section 5.5
2. Unitary operators can be used to change the basis in a vector space, Section 5.7
3. Evolution operators are unitary, Section 5.12
4. Some types of symmetry operators are unitary, Section 5.13

5.5 Properties of Unitary Matrices

The eigenvalues and eigenvectors of unitary matrices have some special properties.

The eigenvalues of a unitary matrix must be unimodular. If U is unitary, then $UU^\dagger = I$. Thus, if

$$U|v\rangle = \lambda|v\rangle \tag{5.5.1}$$

then also

$$\langle v|U^\dagger = \langle v|\lambda^*. \tag{5.5.2}$$

Combining (5.5.1) and (5.5.2) leads to

$$\langle v|v\rangle = \langle v|U^\dagger U|v\rangle = \langle v|\lambda^*\lambda|v\rangle = |\lambda|^2\langle v|v\rangle \tag{5.5.3}$$

Assuming $\lambda \neq 0$, we thus have

$$|\lambda|^2 = 1. \tag{5.5.4}$$

Can the eigenvalue be zero? A matrix with zero as an eigenvalue cannot have an inverse, so the assumption $\lambda \neq 0$ holds automatically for unitary matrices.

Thus, the eigenvalues of a unitary matrix are **unimodular**, that is, they have norm 1, and hence can be written as $e^{i\alpha}$ for some α.

Eigenvectors corresponding to different eigenvalues must be orthogonal. Just as for Hermitian matrices, eigenvectors of unitary matrices corresponding to different eigenvalues must be orthogonal. The argument is similar to the proof for Hermitian matrices in Section 5.3. Suppose that

$$U|v\rangle = e^{i\lambda}|v\rangle, \tag{5.5.5}$$

$$U|w\rangle = e^{i\mu}|w\rangle. \tag{5.5.6}$$

We'd like to evaluate $\langle v|U|w\rangle$ two ways. We know what $U|w\rangle$ is, but not yet what $\langle v|U$ is. So we first compute

$$|v\rangle = U^\dagger U|v\rangle = U^\dagger\left(e^{i\lambda}|v\rangle\right) = e^{i\lambda}\left(U^\dagger|v\rangle\right) \tag{5.5.7}$$

from which it follows that

$$U^\dagger|v\rangle = e^{-i\lambda}|v\rangle \tag{5.5.8}$$

whose conjugate is

$$\langle v|U = \langle v|e^{i\lambda}. \tag{5.5.9}$$

We can now compute

$$\langle v|e^{i\lambda}|w\rangle = \langle v|U|w\rangle = \langle v|e^{i\mu}|w\rangle \tag{5.5.10}$$

so that

$$(e^{i\lambda} - e^{i\mu})\langle v|w\rangle = 0. \tag{5.5.11}$$

Thus, if $e^{i\lambda} \neq e^{i\mu}$, $|v\rangle$ must be orthogonal to $|w\rangle$.

As with Hermitian matrices, this argument can be extended to the case of repeated eigenvalues; it is always possible to find an orthonormal basis of eigenvectors for any unitary matrix.

5.6 Projection Operators

A special class of operators, called **projection operators**, are particularly useful for finding the component of a vector along a particular direction and for changing basis.

Definition 5.6.1 Projection Operator. A operator P_v that gives the same result when acting on any vector twice in succession as when it acts just once, i.e.

$$P_v^2 = P_v, \tag{5.6.1}$$

is called a **projection operator**. ◊

Bra-Ket Representation of Projection Operators. Given any normalized vector $|v\rangle$, that is, a vector satisfying

$$\langle v|v\rangle = 1, \tag{5.6.2}$$

we can show that a projection operator P_v can be constructed by taking the *outer product*, see Section 3.3, of the vector with its Hermitian adjoint.

$$P_v = |v\rangle\langle v|. \tag{5.6.3}$$

The proof is a straightforward calculation using the norm condition (5.6.2)

$$\begin{aligned} P_v^2 &= (|v\rangle\langle v|)(|v\rangle\langle v|) \\ &= |v\rangle(\langle v|v\rangle)\langle v| \\ &= |v\rangle\langle v| \\ &= P_v. \end{aligned} \tag{5.6.4}$$

Using Projection Operators to Implement Projections. Using methods analogous to (5.6.4), we show that P_v takes $|v\rangle$ to itself, that is,

$$\begin{aligned} P_v|v\rangle &= (|v\rangle\langle v|)|v\rangle \\ &= |v\rangle(\langle v|v\rangle) \\ &= |v\rangle; \end{aligned}$$

and takes any vector w that is orthogonal to v, (i.e. $\langle v|w\rangle = 0$), to zero,

$$\begin{aligned} P_v|w\rangle &= (|v\rangle\langle v|)|w\rangle \\ &= |v\rangle(\langle v|w\rangle) \\ &= 0. \end{aligned}$$

This is what we mean when we say P_v *projects* any vector along $|v\rangle$.

Activity 5.6.1 Matrix Representations of Projection Operators. Find the matrix representation of the projection operators corresponding to the vectors:

$$\begin{aligned} |+\rangle &\doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \\ |+\rangle_y &\doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \\ |+\rangle_9 &\doteq \begin{pmatrix} a \\ be^{i\phi} \end{pmatrix}. \end{aligned}$$

Hint 1. The answer should be a square matrix. If you are getting a positive, real number, you are incorrectly taking the inner-product rather than the outer product. Check the order of your matrices.

Hint 2. Don't forget to complex conjugate when you turn the ket into a bra.

5.7 Change of Basis (Bra-Ket Notation)

Definition 5.7.1 The Completeness Relation. If we have an orthonormal basis $\{|v\rangle, |w\rangle, \dots\}$, the definition of orthonormality tells us that

$$\begin{aligned} \langle v|v\rangle = 1 = \langle w|w\rangle = \dots \ , \\ \langle v|w\rangle = 0 = \dots \ . \end{aligned} \tag{5.7.1}$$

Then, we can build projection operators (see Section 5.6) from this orthonormal basis

$$|v\rangle\langle v|, \qquad |w\rangle\langle w|, \qquad \dots \ . \tag{5.7.2}$$

If we add up all these projections, we obtain the identity matrix, that is,

$$I = |v\rangle\langle v| + |w\rangle\langle w| + \dots \ . \tag{5.7.3}$$

Equation (5.7.3) is called the **completeness relation**. ◊

Question 5.7.2 *Check that (5.7.3) is indeed the identity matrix by having it act on the arbitrary vector* $\alpha|v\rangle + \beta|w\rangle + \dots$.

Using the Identity Matrix to Change Basis. If you know a vector $|\psi\rangle = \alpha|v_i\rangle + \beta|w_i\rangle + \dots$ in some initial basis

$$\{|v_i\rangle, |w_i\rangle, \dots\} \tag{5.7.4}$$

and want to find it in some final basis

$$\{|v_f\rangle, |w_f\rangle, \dots\}, \tag{5.7.5}$$

then just use the strategy *multiply by one in a complicated form*, that is, in this case, act on the vector with the identity matrix in the form (5.7.3). The general calculation goes like this:

Don't be intimidated by the sea of algebra. Just FOIL like mad, rearrange terms, and keep track of which terms are vectors and which are scalars.

$$\begin{aligned}
|\psi\rangle &= I|\psi\rangle \\
&= (|v_f\rangle\langle v_f| + |w_f\rangle\langle w_f| + \dots)\,(\alpha|v_i\rangle + \beta|w_i\rangle + \dots) \\
&= |v_f\rangle\,(\alpha\langle v_f|v_i\rangle + \beta\langle v_f|w_i\rangle + \dots) \\
&\quad + |w_f\rangle\,(\alpha\langle w_f|v_i\rangle + \beta\langle w_f|w_i\rangle + \dots) \\
&\quad + \dots
\end{aligned} \tag{5.7.6}$$

Of course, this method is only useful if you already know, or can quickly find, the change of basis elements, e.g. $\langle v_f|v_i\rangle$, between the initial and final basis vectors.

5.8 Diagonalization: Using Eigenvectors as a Natural Basis

The Eigenvectors of Hermitian Matrices form a Natural Basis. In Section 5.3, we showed that the eigenvectors of Hermitian (and anti-Hermitian) matrices are orthogonal, or in the case of degeneracy, can be chosen to be orthogonal. In Section 5.5, we showed the same for unitary (and anti-unitary) matrices.

A much deeper question is whether an $n \times n$ matrix actually has a full n eigenvectors. The **spectral theorem** guarantees that this is the case for Hermitian, anti-Hermitian, unitary, and anti-unitary matrices, but the proof is well beyond the scope of this book. The technical language for this is that the eigenvectors of these matrices form a **complete set**, i.e. they **span** the entire vector space.

Since eigenvectors can always be normalized, see Section 3.5, we see that the eigenvectors of these special matrices form an orthonormal basis.

The next activity explores one of the important implications of using the eigenvectors as a natural basis.

Activity 5.8.1 Find the Form of a Hermitian Operator in Its Own Eigen-Basis. Consider the Hermitian operator A. In a coordinate system where its eigenvectors are the standard basis (4.5.4), name its components

$$A \doteq \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}. \tag{5.8.1}$$

Show that the eigenvalue/eigenvector equation (4.1.1) requires that the diagonal components are the eigenvalues and the off-diagonal elements are zero.

Hint. One of the eigenvalue/eigenvector equations states that

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \lambda_1 \begin{pmatrix} 1 & 0 \end{pmatrix}. \tag{5.8.2}$$

Compare the left- and right-hand sides of this equation.

In the activity above, you showed that, for the simplest example of a 2×2 matrix, in a coordinate system where the eigenvectors of a Hermitian matrix are the standard basis, the Hermitian matrix is diagonal and its diagonal elements are just the eigenvalues. This result is true, in general, for any size matrix that is Hermitian, anti-Hermitian, unitary, or anti-unitary.

The process of **diagonalization** is the process of changing basis to the natural eigen-basis of such an operator. To actually find the change-of-basis operation requires some algebra (which we will not discuss further here). But scientists often casually say that they are ''diagonalizing'' a matrix when all they really do is state the diagonal matrix that is the result.

To Remember. A Hermitian matrix is diagonal in its own eigen-basis and, in this coordinate system, its eigenvectors are just the standard basis (4.5.4). Many calculations are simplified by using this basis.

5.9 Matrix Decompositions

UNDER CONSTRUCTION

Returning to our special matrices, we have shown that both Hermitian and unitary matrices admit orthonormal basis of eigenvectors. So suppose that

$$M|v\rangle = \lambda|v\rangle, M|w\rangle = \mu|w\rangle, ... \tag{5.9.1}$$

where $|v\rangle$, $|w\rangle$, ... satisfy (5.7.1). Then (5.7.3) is satisfied, and a similar argument shows that

$$M = \lambda|v\rangle\langle v| + \mu|w\rangle\langle w| + ... \ , \tag{5.9.2}$$

so that we can expand any Hermitian or unitary matrix in terms of its eigenvalues and the projection operators formed from its eigenvectors.

5.10 Parameterization of Hermitian and Unitary Matrices

Any 2×2 Hermitian matrix, M, can be written in the form

$$M = \begin{pmatrix} t+z & x-iy \\ x+iy & t-z \end{pmatrix} \tag{5.10.1}$$

with $x, y, z, t \in \mathbb{R}$. Looking at the matrix coefficients of these variables, we can write

$$M = t\, I + x\, \sigma_x + y\, \sigma_y + z\, \sigma_z \tag{5.10.2}$$

thus defining the three matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{5.10.3}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{5.10.4}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{5.10.5}$$

which are known as the **Pauli matrices**. The Pauli matrices $\{\sigma_m\}$ have several interesting properties. First of all, each Pauli matrix squares to the identity matrix, is tracefree, and of course is Hermitian:

$$\sigma_m^2 = I, \tag{5.10.6}$$
$$tr(\sigma_m) = 0, \tag{5.10.7}$$
$$\sigma_m^\dagger = \sigma_m. \tag{5.10.8}$$

Also of interest is that these matrices anticommute, and that the product of any two is the third, for instance:

$$\sigma_x\sigma_y = i\,\sigma_z = -\sigma_y\sigma_x. \tag{5.10.9}$$

Thus, any 2×2 Hermitian matrix can be written as a real linear combination of the Pauli matrices and the identity matrix.

What about 2×2 unitary matrices? Now we must have $MM^\dagger = I$, that is,

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix} = \begin{pmatrix} |a|^2+|b|^2 & ac^*+bd^* \\ ca^*+db^* & |c|^2+|d|^2 \end{pmatrix} = I. \tag{5.10.10}$$

The normalization conditions

$$|a|^2 + |b|^2 = 1 = |c|^2 + |d|^2 \tag{5.10.11}$$

allow us to write

$$a = e^{i\alpha}\cos\theta, \tag{5.10.12}$$
$$b = e^{i\beta}\sin\theta, \tag{5.10.13}$$
$$c = e^{i\gamma}\sin\phi, \tag{5.10.14}$$
$$d = e^{i\delta}\cos\phi, \tag{5.10.15}$$

where we can assume that $\theta, \phi \in [0, \frac{\pi}{2}]$. The remaining condition becomes

$$0 = ac^* + bd^* = e^{i(\alpha-\gamma)}\cos\theta\sin\phi + e^{i(\beta-\delta)}\sin\theta\cos\phi \tag{5.10.16}$$

which forces in general

$$\tan\theta = \tan\phi, \tag{5.10.17}$$
$$e^{i(\alpha-\gamma)} = -e^{i(\beta-\delta)} \tag{5.10.18}$$

(with the second condition unnecessary if $\theta = 0$ or $\theta = \frac{\pi}{2}$), so that

$$\theta = \phi, \tag{5.10.19}$$
$$\alpha + \delta = \beta + \gamma - \pi. \tag{5.10.20}$$

Some special cases are $\alpha = 0 = \delta$, $\beta = \frac{\pi}{2} = \gamma$, corresponding to

$$U_x = \begin{pmatrix} \cos\theta & i\sin\theta \\ i\sin\theta & \cos\theta \end{pmatrix}, \tag{5.10.21}$$

$\alpha = 0 = \delta$, $\beta = 0$, $\gamma = \pi$, corresponding to

$$U_y = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \tag{5.10.22}$$

and $\theta = 0$, $\delta = \alpha$, corresponding to

$$U_z = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}, \tag{5.10.23}$$

where we have replaced α by θ for consistency.

5.11 Matrix Exponentials

How do you exponentiate matrices?

Recall the power series

$$e^{i\theta} = 1 + i\theta - \frac{\theta^2}{2!} - i\frac{\theta^3}{3!} + ... \tag{5.11.1}$$

which can famously be used to prove Euler's formula, namely

$$e^{i\theta} = \cos\theta + i\sin\theta. \tag{5.11.2}$$

We can use this same strategy to exponentiate matrices, by using the corresponding power series. We therefore define

$$e^{iM\theta} = I + iM\theta - \frac{M^2\theta^2}{2!} - i\frac{M^3\theta^3}{3!} + ... \tag{5.11.3}$$

Let's consider some special cases. First consider a matrix M satisfying $M^2 = I$, such as the *Pauli matrices*, see Section 5.10. For any such matrix, we have

$$\begin{aligned} e^{iM\theta} &= I + iM\theta - \frac{\theta^2}{2!} - i\frac{M\theta^3}{3!} + ... \\ &= I\cos\theta + iM\sin\theta \end{aligned} \tag{5.11.4}$$

For example,

$$e^{i\sigma_x\theta} = I\cos\theta + i\sigma_x\sin\theta = \begin{pmatrix} \cos\theta & i\sin\theta \\ i\sin\theta & \cos\theta \end{pmatrix} = U_x, \tag{5.11.5}$$

and similarly

$$e^{i\sigma_y\theta} = U_y, \tag{5.11.6}$$

$$e^{i\sigma_z\theta} = U_z. \tag{5.11.7}$$

In fact, exponentiating a Hermitian matrix in this way always yields a unitary matrix, since

$$\left(e^{iM\theta}\right)^\dagger = e^{-iM^\dagger\theta}, \tag{5.11.8}$$

as can be verified by working term-by-term with the power series. The converse is also true; any unitary matrix U can be written as $e^{iM\theta}$ for some Hermitian matrix M.

Remarkably, the eigenvector decompositions derived in the last section behave very nicely under exponentiation, as we now show.

Let M be Hermitian, and recall that we can expand M in terms of its eigenvectors and eigenvalues as

$$M = \lambda|v\rangle\langle v| + \mu|w\rangle\langle w| + ... \ . \tag{5.11.9}$$

Notice that

$$M^2 = \lambda^2|v\rangle\langle v| + \mu^2|w\rangle\langle w| + ... \ . \tag{5.11.10}$$

since all cross terms cancel, and since each projection matrix squares to itself. Furthermore, recall that the projections add up to the identity matrix, that is,

$$I = |v\rangle\langle v| + |w\rangle\langle w| + ... \ , \tag{5.11.11}$$

Putting this all together, we see that

$$e^{iM\theta} = e^{i\lambda\theta}|v\rangle\langle v| + e^{i\mu\theta}|w\rangle\langle w| + \dots \,, \tag{5.11.12}$$

which shows explicitly how to relate the decompositions of Hermitian matrices and their corresponding unitary matrices. This remarkable result is much less surprising when expanded in terms of the given orthonormal basis, in which case M is diagonal, so that exponentiating the matrix is just exponentiating each of the eigenvalues.

5.12 Evolution Equation

The simplest non-trivial ode is the first-order linear ode with constant coefficients:

$$\frac{d}{dx} f(x) = a f(x) \tag{5.12.1}$$

with solution:

$$f(x) = f(0)\, e^{ax} \tag{5.12.2}$$

We can generalize this equation to apply to solutions which are exponentials of matrices (Section 5.11), i.e.:

$$M(x) = M(0) e^{Ax} \tag{5.12.3}$$

is a solution of:

$$\frac{d}{dx}\, M(x) = A\, M(x) \tag{5.12.4}$$

where A is a suitable constant matrix. (Show that if A is anti-Hermitian, then $M(x)$ is unitary.)

Example Problem: Find the matrix differential equation that has the solution:

$$|\psi(x,t)\rangle = |\psi(x,0)\rangle\, e^{i\frac{Ht}{\hbar}} \tag{5.12.5}$$

where H is Hermitian. Do you recognize your differential equation?

5.13 Symmetry Operations

COMING SOON

Chapter 6

Differentials

6.1 Review of Single Variable Differentiation

Theory. Differentiation is about how small changes in one quantity influence other quantities. This "ratio of small changes" viewpoint is often helpful in setting up problems involving differentiation, and will be especially useful later for partial derivatives.

For example, how do you determine how fast are you going? If you know how far you went during a given time interval, you can divide these quantities to determine your average speed during that interval. Repeat this computation over shorter and shorter time periods. Those are still, strictly speaking, average speeds, but they are better and better approximations to your instantaneous rate of change.

Equivalently, draw a graph showing your position as a function of time. If you connect any two points on this graph, the horizontal "distance" between them represents the amount of time it took to get from one to the other, and the vertical "distance" between them represents how far apart they are. Dividing these two quantities again yields your average speed for that part of your journey, which is also clearly the slope of the *secant line* connecting the two points. Repeat this computation over shorter and shorter time periods, and the slope of the secant line becomes a better and better approximation to the slope of the *tangent line*, which gives the instantaneous rate of change.

In either case, the construction outlined above yields your speed *at a single point*, but you can repeat the construction at every point. *Derivatives are functions!*

Limits. The constructions above are usually expressed in terms of *limits*. If your position is given by $y = 2x^2$, then your speed can be computed by calculating

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x} = \lim_{\Delta x \to 0} \frac{2(x + \Delta x)^2 - 2x^2}{\Delta x} = 4x \tag{6.1.1}$$

where some algebra is required to obtain the final answer. The notation $\frac{dy}{dx}$ emphasizes that derivatives are built from ratios of the small quantities Δy and Δx. Note the dependence on x; your speed is not constant.

Practice. Limits are rarely used when computing derivatives in practice. Instead, one derives and then typically memorizes a few basic rules, such as

the *Power Rule*, which says that

$$\frac{d}{dx}(x^n) = nx^{n-1} \tag{6.1.2}$$

and the *Product Rule*, which says that

$$\frac{d}{dx}(fg) = f\frac{dg}{dx} + g\frac{df}{dx} \tag{6.1.3}$$

where f and g are arbitrary functions of x, that is, $f = f(x)$ and $g = g(x)$.

6.2 Derivative Notation

There are two traditional notations for derivatives, which you have likely already seen.

Newton/Lagrange/Euler: In this notation, the primary objects are *functions*, such as $f(x) = x^2$, and derivatives are written with a prime, as in $f'(x) = 2x$.

This notation is often referred to as "Newtonian", but Newton actually used dots rather than primes, and used t rather than x as the independent variable. The use of primes and x is often attributed to Lagrange, but was in fact introduced by Euler.

Leibniz: In this notation, due to Leibniz, the primary objects are *relationships*, such as $y = x^2$, and derivatives are written as a ratio, as in $\frac{dy}{dx} = 2x$.

These notations extend naturally to higher derivatives. We summarize the disscussion so far as follows:

Notation 6.2.1 Derivatives. There are several different notations for derivatives in common use. You should be comfortable with all of them. Leibniz's notation for derivatives is:

$$\frac{dy}{dx}, \qquad \frac{d^2y}{dx^2}, \qquad \frac{d^3y}{dx^3}, \qquad \dots \qquad \frac{d^ny}{dx^n} \tag{6.2.1}$$

Lagrange's notation for the same derivatives is: [1]

$$y', \qquad y'', \qquad y''', \qquad \dots \qquad y^{(n)} \tag{6.2.2}$$

It is also common to set $y = f(x)$ and write $f'(x)$ instead of y', etc.

Newton used *dots* instead of *primes* (and t as the independent variable, rather than x):

$$\dot{y}, \qquad \ddot{y}, \qquad \dots \qquad y^{(n)} \tag{6.2.3}$$

All of these notations work fine for functions of a single variable. However, Leibniz notation is better suited to situations involving many quantities that are changing, both because it keeps explicit track of which derivative you took ("with respect to x"), and because it emphasizes that derivatives are ratios. Among other things, this helps you get the units right; mph are a ratio of miles to hours!

6.3 Thick Derivatives

In Section 6.1, we briefly discussed representing derivatives *symbolically* (as ratios), *graphically* (as slopes), and even *verbally* (as the ratio of small quantities).

[1] This notation was originally introduced by Euler.

What about *numerically* or *experimentally*? [1]

Suppose you record your position every few minutes. You can make a table of your data, showing times and positions. How fast were you going?

Well, you can divide the various distances traveled by the time it took, but the results are clearly average speeds for each interval. What if you were to record your position every few seconds? Every few microseconds?

Mathematicians would argue that this question is still poorly posed: Since you only have discrete, numerical data, no limits can be taken, so you can only ever compute average speeds. On the other hand, in everyday circumstances the accuracy obtained with data taken every few microseconds is surely sufficient.

In the real world, the important question is not whether the computation yields an average speed or an instantaneous speed, but rather whether the average is "good enough", where of course what's good enough depends on the context.

Rather than engage in a pedantic discussion of whether one can in principle compute derivatives from numerical or experimental data, we choose to embrace such computations due to their importance in applications. We therefore introduce the concept of "thick" derivatives to encompass both instantaneous rates of change and average rates of change that are "good enough". Again, this notion depends on the context; a detailed analysis properly belongs to the fields of numerical analysis and data analysis. Nonetheless, we will not quibble about referring to the results of measurements over suitably small intervals as "derivatives".

For further discussion, see [2].

6.4 Differentials

Both of the derivative notations described in Section 6.2 distinguish between dependent quantities ($f(x)$ or y) and the independent variable (x). However, in the real world one doesn't always know in advance which variables are independent. We therefore go one step further, and express derivatives in terms of *differentials*.

[1] We would argue that these are not quite the same thing, since experimental computations are limited by measurement error, whereas numerical computations are limited by roundoff error, a fundamentally different concept.

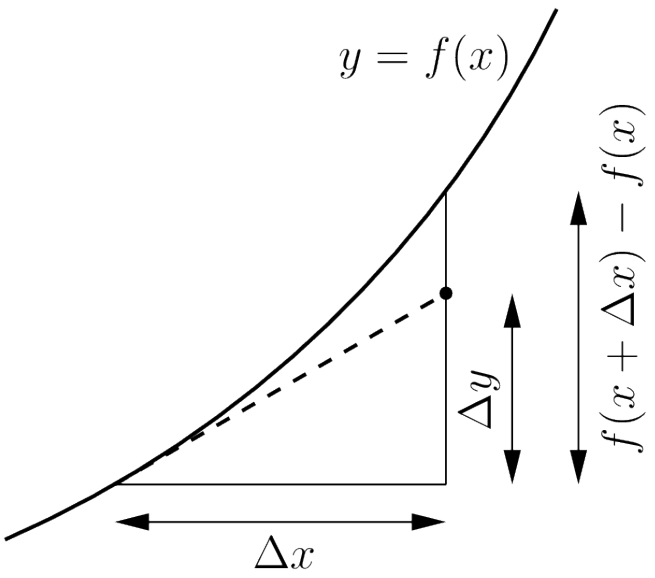


Figure 6.4.1 Linear approximation using the tangent line.

The tangent line to the graph of $y = f(x)$ at the point (x_0,y_0) is given by

$$y - y_0 = m\,(x - x_0) \tag{6.4.1}$$

where the slope m is of course just the derivative $\frac{df}{dx}\big|_{x=x_0}$. It is tempting to rewrite the equation of the tangent line as

$$\Delta y = \frac{df}{dx}\Delta x \tag{6.4.2}$$

which is also used for linear approximation in the form

$$\Delta f = f(x + \Delta x) - f(x) \approx \frac{df}{dx}\Delta x \tag{6.4.3}$$

as shown in Figure 6.4.1. Regarding Δx as small, we rewrite (6.4.3) in the form

$$df = \frac{df}{dx}\,dx \tag{6.4.4}$$

where the **differential** df can be interpreted as the corresponding small change in f.

The intuitive idea behind differentials is to consider the small quantities "dy" and "dx" separately, with the derivative $\frac{dy}{dx}$ denoting their relative rate of change. So rather than either of the traditional expressions for derivatives (see Section 6.2), if $y = x^2$ we write

$$dy = 2x\,dx. \tag{6.4.5}$$

More generally, if y is any function of x, then the *derivative* $\frac{dy}{dx}$ relates the *differentials* dy and dx via

$$dy = \frac{dy}{dx}dx. \tag{6.4.6}$$

You can safely think of (6.4.5) as a sufficiently small quantity, or as the numerator of Leibniz notation, or as shorthand for a limit argument, or in terms of differential forms, or nonstandard analysis, or ...; it doesn't matter, they all give the same equations.

6.5 Rules for Differentials

We can eliminate y from (6.4.5) by writing

$$d(x^2) = 2x\,dx, \tag{6.5.1}$$

and we can go even further by replacing the ubiquitous variable x by any physical or geometric quantity, such as u. The beauty of this approach is that differentiation is easy once you have convinced yourself of a few basic rules.

Let's start with some simple functions. For instance, the power rule for derivatives says that

$$\frac{d}{du}(u^n) = nu^{n-1} \tag{6.5.2}$$

which in differential notation becomes $d(u^n) = nu^{n-1}\,du$.

Notation. We use u and later v to denote *any* quantity. It might be the case that $u = x$, or that $u = f(x)$, or that $u = f(x, y)$, or that u depends on other quantities. it doesn't matter.

Usage. "Taking the differential" or "zapping with d" is an *operation*; d itself is an *operator*, that acts on functions.

Applying this construction to the derivatives of elementary functions, we obtain the basic differentiation formulas in differential form, namely:

$$\begin{aligned}
d\left(u^n\right) &= nu^{n-1}\,du,\\
d\left(e^u\right) &= e^u\,du,\\
d(\sin u) &= \cos u\,du,\\
d(\cos u) &= -\sin u\,du,\\
d(\ln u) &= \frac{1}{u}\,du,\\
d(\tan u) &= \frac{1}{\cos^2 u}\,du.
\end{aligned}$$

So how do we use these formulas to compute derivatives?

6.6 Properties of Differentials

Both derivatives and differentials (and, in fact, all forms of differentiation that you may learn about in the future) satisfy two basic properties: linearity and the product rule.

Linearity. You probably use a property of ordinary derivatives, called **linearity**, without even thinking about it. Linearity meansthat the derivative of a sum is the sum of the derivatives (distributivity), and constants pull through the derivative. For example:

$$\frac{d}{dx}(3x^2 + e^{kx}) = \frac{d}{dx}(3x^2) + \frac{d}{dx}(e^{kx}) = 6x + ke^{kx}. \tag{6.6.1}$$

This same property applies to differentials. If u and v are any two quantities, then linearity says that

$$d(au + bv) = a\,du + b\,dv \tag{6.6.2}$$

where a and b are constants.

In these expressions, u and v may or may not be related. For example, if $u = x^2$ and $v = e^{kx}$ both depend on x, then

$$\begin{aligned} d(3x^2 + e^{kx}) &= d(3x^2) + d(e^{kx}), \\ &= 6x\,dx + ke^{kx}\,dx = (6x + ke^{kx})\,dx. \end{aligned} \tag{6.6.3}$$

Product Rule. The product rule for differentials follows the same pattern as the product rule for ordinary derivatives, namely

$$d(uv) = u\,dv + v\,du. \tag{6.6.4}$$

As an example, consider the *ideal gas law*

$$pV = nRT \tag{6.6.5}$$

relating the pressure p, volume V, and temperature T of an ideal gas, where R is a physical constant, and n is the number of moles of gas, which we will assume remains constant in this example. "Zapping" (6.6.5) with d, the product rule yields

$$d(pV) = p\,dV + V\,dp = nR\,dT. \tag{6.6.6}$$

Chain Rule. In Leibniz notation, the chain rule for ordinary derivatives is:

$$\frac{dy}{dx} = \frac{dy}{du}\,\frac{du}{dx}. \tag{6.6.7}$$

From the point of view of the ratio of small changes, (6.6.7) is just a statement about the ordinary rules for manipulating fractions.

For differentials, the chain rule becomes:

$$dy = \frac{dy}{du}\,\frac{du}{dx}\,dx. \tag{6.6.8}$$

We are assuming that dy and dx are "small enough" that we can treat the relationships between y and u and between u and x as linear, so the two rates of change in (6.6.8) just multiply.

The product of two rates of change in (6.6.8) is like doing a double change of units.

$$N\frac{km}{hr} = N\frac{km}{hr} \times 1000\frac{m}{km} \times \frac{1}{3600}\frac{hr}{sec} = N\frac{1000}{3600}\frac{m}{sec}$$

Suppose you want to find the derivative of $Q = \ln\sin(\theta^2)$. How many functions are there here? Three; let's consider each in turn.

The first, "outer" function is the logarithm. Logarithm of what? Give it a name! So we set $u = \sin(\theta^2)$, and similarly $v = \theta^2$. We now have $Q = \ln u$ and $u = \sin v$, so that

$$dQ = d(\ln u) = \frac{1}{u}du = \frac{1}{u}\cos v\,dv = \frac{\cos v}{u}2\theta\,d\theta. \tag{6.6.9}$$

Dividing by $d\theta$ yields an expression for the derivative of Q with respect to θ, namely

$$\frac{dQ}{d\theta} = \frac{\cos v}{u}2\theta = 2\theta\cot(\theta^2) \tag{6.6.10}$$

where it is customary to expand u and v in terms of θ in the final answer.

This process is often described as "peeling an onion", with each layer corresponding to a different function, represented here by a different variable.

Inverse Functions. The rule for the derivative of inverse functions is

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

which in differential notation becomes

$$dx = \frac{1}{dy/dx}\, dy.$$

As an example, we derive the derivative formula for logarithms from that for the exponential function. If $u = \ln v$, then $v = e^u$; both of these equations represent the same relationship between u and v. If we don't know how to differentiate the first expression, we can differentiate the second, yielding

$$dv = d(e^u) = e^u du = v\, du \tag{6.6.11}$$

from which it follows immediately that

$$du = \frac{1}{v} dv \tag{6.6.12}$$

which was the desired derivative formula for the inverse of exponentation. Yes, it's that easy!

Implicit Differentiation. Implicit differentiation can be accomplished in differential notation simply by "zapping" every term in an equation with d, that is, by taking the differential (not the derivative) of both sides of the equation, using the rules above.

For example, consider the problem of finding the slope of the tangent line to a circle at an arbitrary point. We have

$$x^2 + y^2 = a^2 \tag{6.6.13}$$

with a constant, and zapping each term with d yields

$$2x\, dx + 2y\, dy = 0 \tag{6.6.14}$$

from which it is easy to derive

$$\frac{dy}{dx} = -\frac{x}{y} \tag{6.6.15}$$

which can then be evaluated at the desired point.

Note the shift in emphasis when using differentials to compute derivatives in these examples:

- We didn't solve for y (or x); no attempt was made to identify dependent and independent variables.
- At each stage, "zapping" with d produced a new term with d, which is a differential, not a derivative.
- The physical answer is almost never a differential, but rather a derivative, namely the ratio of two differentials.

6.7 Substitution

The formulas in differential form given at the end of Section 6.5 not only summarize the basic differentiation formulas, but also the basic integration formulas! In each case, one can integrate both sides of the expression, then use the Fundamental Theorem of Calculus, which says that

$$\int df = f \tag{6.7.1}$$

which can be interpreted as a statement about antiderivatives. For example, knowing that

$$d(u^n) = nu^{n-1}\,du \tag{6.7.2}$$

immediately tells us that

$$u^n = \int d(u^n) = \int nu^{n-1}\,du \tag{6.7.3}$$

which is normally rewritten in the form

$$\int u^m\,du = \frac{u^m}{m+1} \tag{6.7.4}$$

where $m = n + 1$.

Some of the differentiation rules introduced in Section 6.6 also lead to integration rules. For example, the product rule in the form

$$d(uv) = u\,dv + v\,du \tag{6.7.5}$$

immediately yields

$$uv = \int d(uv) = \int u\,dv + \int v\,du \tag{6.7.6}$$

which is normally rewritten in the form

$$\int v\,du = uv - \int u\,dv \tag{6.7.7}$$

where it is known as **integration by parts**.

But the most important of these integration rules is the analog of the chain rule. Multiplying both sides of

$$du = \frac{du}{dx}\,dx \tag{6.7.8}$$

by an arbitrary function f and then integrating yields first

$$f\,du = f\,\frac{du}{dx}\,dx \tag{6.7.9}$$

and then

$$\int f\,du = \int f\,\frac{du}{dx}\,dx \tag{6.7.10}$$

which is the technique known as **substitution**. [1] For example, to evaluate the integral

$$Q = \int \sin^2\theta\cos\theta\,d\theta \tag{6.7.11}$$

it is enough to notice that $d\sin\theta = \cos\theta\,d\theta$, so that the integral becomes

$$Q = \int \sin^2\theta\,d(\sin\theta) = \frac{1}{3}\sin^3\theta \tag{6.7.12}$$

where the substitution $u = \sin\theta$ has been made implicitly.

[1] This technique is often referred to as "u-substitution" even when there is no variable named u.

6.8 Differentials: Summary

We summarize here both the basic differentiation formulas from Section 6.5 and the fundamental rules from Section 6.6, in differential form. We have:

$$\begin{aligned} d\left(u^n\right) &= nu^{n-1}\,du, \\ d\left(e^u\right) &= e^u\,du, \\ d(\sin u) &= \cos u\,du, \\ d(\cos u) &= -\sin u\,du, \\ d(\ln u) &= \frac{1}{u}\,du, \\ d(\tan u) &= \frac{1}{\cos^2 u}\,du, \\ d(u+cv) &= du + c\,dv, \\ d(uv) &= u\,dv + v\,du, \\ d\left(\frac{u}{v}\right) &= \frac{v\,du - u\,dv}{v^2}, \end{aligned}$$

where c is a constant. Each of these rules can be reinterpreted as a *derivative* rule by deviding both sides by du, and as an *integration* rule by integrating both sides (and using the Fundamental Theorem of Calculus in the form $\int df = f$).

We have added the *quotient rule* at the end of this list, which can be obtained quickly from the power and product rules by writing $\frac{u}{v} = u\frac{1}{v}$. (Similarly, any one rule for differentiating a trigonometric function can be used to derive the others, and, as we saw in Section 6.6, the rule for the exponential function can be used to derive the rule for logarithms – or vice versa. Nonetheless, each of these rules is used often enough that it is helpful to include them all.)

We reiterate that there is no need to add the chain rule to this list, nor the rules for inverse functions or implicit differentiation.

Finally, a nice mnemonic to help you avoid mixing up differentials with derivatives, especially at first, is to think of terms involving d as *small*. Derivatives are the ratios of small quantities, but they are not themselves small. And each term in an equation must have the same character, big or small. Put differently, the ds must balance; (infinitesimally) small quantities can never be equal to (finite) big quantities.

6.9 The Multivariable Differential

In Section 6.4, we considered the tangent line to the graph of a function f of one variable. What if f is a function of more than one variable?

Consider the tangent plane to the graph of $z = f(x, y)$ at the point (x_0,y_0,z_0). What is the height difference Δz between two points on the tangent plane? Hold a piece of paper at an arbitrary angle in front of you, and imagine moving on it first to the right, then directly forwards. How high did you go? The sum of the height differences in each step. How big are these height differences? As above, they are precisely the horizontal distance traveled multiplied by the appropriate slope.

In other words, the equation of the tangent plane is given by

$$z - z_0 = m_x\,(x - x_0) + m_y\,(y - y_0) \tag{6.9.1}$$

where m_x and m_y are the slopes in the x and y directions. But these slopes are (by definition) the *partial derivatives* of f with respect to x and y (at the given point).

In the xy-plane, the partial derivative of f with respect to x is written as $\frac{\partial f}{\partial x}$, and means "the derivative of f with respect to x *with y held constant*". In some contexts, it is necessary to state explicitly what variables are being held constant, in which case this partial derivative may be written as $\left(\frac{\partial f}{\partial x}\right)_y$. Make sure you distinguish between d and ∂; writing the letter "d" so that it looks like a ∂ is not correct mathematics.

Returning to our graph, we can therefore write the equation of the tangent plane as

$$\Delta z = \frac{\partial f}{\partial x}\Delta x + \frac{\partial f}{\partial y}\Delta y \tag{6.9.2}$$

which leads to the following expression for the differential of f

$$df = \frac{\partial f}{\partial x}\,dx + \frac{\partial f}{\partial y}\,dy \tag{6.9.3}$$

which again can be thought of as the small change in f corresponding to small changes in x and y. Similar expressions hold for functions of more than two variables.

Notice that there is nothing special about the variable names x and y. If f is a function of any two parameters α and β, then we have a formula equivalent to (6.9.3)), namely

$$df = \frac{\partial f}{\partial \alpha}\,d\alpha + \frac{\partial f}{\partial \beta}\,d\beta \tag{6.9.4}$$

In particular, it is not necessary for α and β to have the same dimensions.

Chapter 7

Chain Rule

7.1 Chain Rule

One advantage of working with differentials is that the chain rule becomes automatic. For example, if you know the temperature T of a metal girder as a function of position x, and you know your position as a function of time t, then you can of course obtain temperature as a function of time by substitution. The resulting expression could be differentiated to determine how quickly the temperature at your location is changing as you move along the girder. But you could also use the chain rule, starting from the differential expression

$$dT = \frac{dT}{dx}\,dx \tag{7.1.1}$$

and then "dividing" by dt to obtain

$$\frac{dT}{dt} = \frac{dT}{dx}\,\frac{dx}{dt}. \tag{7.1.2}$$

Equation (7.1.2) is the traditional statement of the *single-variable chain rule*.

Functions of several variables can be handled just as easily. For example, if you know the termperature T as a function of position in space, and you know your position as a function of time, then a similar computation would start with

$$dT = \frac{\partial T}{\partial x}\,dx + \frac{\partial T}{\partial y}\,dy + \frac{\partial T}{\partial z}\,dz \tag{7.1.3}$$

and then "divide" by dt to obtain

$$\frac{dT}{dt} = \frac{\partial T}{\partial x}\,\frac{dx}{dt} + \frac{\partial T}{\partial y}\,\frac{dx}{dt} + \frac{\partial T}{\partial z}\,\frac{dz}{dt}. \tag{7.1.4}$$

Now suppose that your position in space depends on latitude and longitude, rather than on time. So

$$dx = \frac{\partial x}{\partial \theta}\,d\theta + \frac{\partial x}{\partial \phi}\,d\phi \tag{7.1.5}$$

where (θ,ϕ) are spherical coordinates, with similar expressions holding for dy and dz. Suppose you want to know how the temperature changes as you walk along a line of constant latitude, that is, with ϕ held constant. We can substitute (7.1.5) into (7.1.3), along with the similar expressions for dy and dz, obtaining

$$dT = \frac{\partial T}{\partial x}\left(\frac{\partial x}{\partial \theta}\,d\theta + \frac{\partial x}{\partial \phi}\,d\phi\right) + \frac{\partial T}{\partial y}\left(\frac{\partial y}{\partial \theta}\,d\theta + \frac{\partial y}{\partial \phi}\,d\phi\right) + \frac{\partial T}{\partial z}\left(\frac{\partial z}{\partial \theta}\,d\theta + \frac{\partial z}{\partial \phi}\,d\phi\right)$$

$$= \left(\frac{\partial T}{\partial x}\frac{\partial x}{\partial \theta} + \frac{\partial T}{\partial y}\frac{\partial y}{\partial \theta} + \frac{\partial T}{\partial z}\frac{\partial z}{\partial \theta}\right) d\theta + \left(\frac{\partial T}{\partial x}\frac{\partial x}{\partial \phi} + \frac{\partial T}{\partial y}\frac{\partial y}{\partial \phi} + \frac{\partial T}{\partial z}\frac{\partial z}{\partial \phi}\right) d\phi.$$

But we also have

$$dT = \frac{\partial T}{\partial \theta}\, d\theta + \frac{\partial T}{\partial \phi}\, d\phi \tag{7.1.6}$$

and by comparing coefficients we obtain

$$\frac{\partial T}{\partial \theta} = \frac{\partial T}{\partial x}\frac{\partial x}{\partial \theta} + \frac{\partial T}{\partial y}\frac{\partial y}{\partial \theta} + \frac{\partial T}{\partial z}\frac{\partial z}{\partial \theta} \tag{7.1.7}$$

as well as a similar expression for $\frac{\partial T}{\partial \phi}$.

Equation (7.1.7) is the traditional statement of the *multivariable chain rule*. You can easily reconstruct this expression from (7.1.3) by "dividing" by $d\theta$, so long as you remember to replace ordinary derivatives by partial derivatives.

7.2 Chain Rule via Tree Diagrams

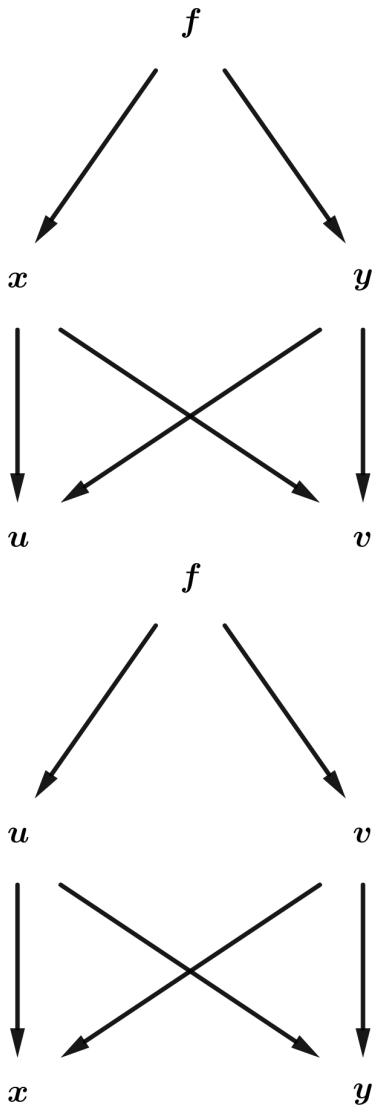


Figure 7.2.1 Tree diagrams relating x, y with u, v.

Suppose $f = f(x, y)$. Then of course

$$df = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy$$

where the subscripts keep track of which variables are being held constant when taking partial derivatives. If $x = x(u, v)$, $y = y(u, v)$, then

$$dx = \left(\frac{\partial x}{\partial u}\right)_v du + \left(\frac{\partial x}{\partial v}\right)_u dv$$

with a similar expression holding for dy. Combining these expressions and rearranging terms, we obtain

$$\begin{aligned} df = &\left(\left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial u}\right)_v + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial u}\right)_v\right) du \\ &+ \left(\left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial v}\right)_u + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial v}\right)_u\right) dv. \end{aligned}$$

But we also know that

$$df = \left(\frac{\partial f}{\partial u}\right)_v du + \left(\frac{\partial f}{\partial v}\right)_u dv.$$

Setting $v =$ constant, we obtain

$$\left(\frac{\partial f}{\partial u}\right)_v = \left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial u}\right)_v + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial u}\right)_v \tag{7.2.1}$$

with a similar expression holding for the derivative of f with respect to v.

An easy way to remember such formulas is to use a *tree diagram*, as shown in the first diagram in Figure 7.2.1. To use a tree diagram, determine which derivative you want to take, in this case the derivative of f with respect to u. Now follow all possible paths from f to u, with each arrow corresponding to a derivative of the "top" quantity with respect to the "bottom" quantity, and where in each case the variable(s) *not* pointed to by the arrow are to be held constant.

However, one often wants to know how to express the derivatives of f with respect to x and y in terms of its derivatives with respect to u and v, rather than the other way around. The argument in this case is the same, with the roles of (x,y) and (u,v) reversed, as in the tree diagram in the second diagram in Figure 7.2.1. This construction results in

$$\left(\frac{\partial f}{\partial x}\right)_y = \left(\frac{\partial f}{\partial u}\right)_v \left(\frac{\partial u}{\partial x}\right)_y + \left(\frac{\partial f}{\partial v}\right)_u \left(\frac{\partial v}{\partial x}\right)_y \tag{7.2.2}$$

with a similar expression for the derivative of f with respect to y. When comparing (7.2.2) with (7.2.1), it is important to realize that $\left(\frac{\partial x}{\partial u}\right)_v$ and $\left(\frac{\partial u}{\partial x}\right)_y$ are not necessarily reciprocals of each other. [1]

Finally, it is possible to reinterpret (7.2.2) as a statement about derivative operators, rather than derivatives, simply by removing f. Thus,

$$\left(\frac{\partial}{\partial x}\right)_y = \left(\frac{\partial u}{\partial x}\right)_y \left(\frac{\partial}{\partial u}\right)_v + \left(\frac{\partial v}{\partial x}\right)_y \left(\frac{\partial}{\partial v}\right)_u \tag{7.2.3}$$

[1] It turns out that the partial derivatives relating (x, y) to (u, v) and vice versa can be viewed as the components of a matrix, and that the two matrices are inverses of each other.

where we have reordered the terms slightly. When using such expressions, you will often need to express the derivatives on the RHS in terms of u and v alone, rather than in terms of x and y. Having done so, it is possible to use these expressions to determine higher-order derivative operators as well, such as the Laplacian.

7.3 Applications of Chain Rule

When differentiating functions of several variables, it is essential to keep track of which variables are being held fixed. As a simple example, suppose

$$f = 2x + 3y \tag{7.3.1}$$

for which it seems clear that

$$\frac{\partial f}{\partial x} = 2 \tag{7.3.2}$$

But suppose we know that

$$y = x + z \tag{7.3.3}$$

so that

$$f = 2x + 3(x + z) = 5x + 3z \tag{7.3.4}$$

from which it seems equally clear that

$$\frac{\partial f}{\partial x} = 5 \tag{7.3.5}$$

In such cases, we adopt a more precise notation, and write

$$\left(\frac{\partial f}{\partial x}\right)_y = 2, \qquad \left(\frac{\partial f}{\partial x}\right)_z = 5, \tag{7.3.6}$$

where the subscripts indicate the variable(s) being held constant.

We can now prove two useful identities about partial derivatives. Suppose that we know a relationship such as $F(x, y, z) = 0$, so that any of x, y, z can in principle be expressed in terms of the other two variables. Then we have

$$\begin{aligned} dz &= \left(\frac{\partial z}{\partial x}\right)_y dx + \left(\frac{\partial z}{\partial y}\right)_x dy \\ &= \left(\frac{\partial z}{\partial x}\right)_y dx + \left(\frac{\partial z}{\partial y}\right)_x \left[\left(\frac{\partial y}{\partial z}\right)_x dz + \left(\frac{\partial y}{\partial x}\right)_z dx\right] \\ &= \left[\left(\frac{\partial z}{\partial x}\right)_y + \left(\frac{\partial z}{\partial y}\right)_x \left(\frac{\partial y}{\partial x}\right)_z\right] dx + \left(\frac{\partial z}{\partial y}\right)_x \left(\frac{\partial y}{\partial z}\right)_x dz. \end{aligned} \tag{7.3.7}$$

Since x and z are independent, the coefficients of dx and dz on each side of (7.3.7) must separately agree. (Equivalently, set x and z in turn equal to constants.) Thus,

$$\begin{aligned} \left(\frac{\partial z}{\partial y}\right)_x \left(\frac{\partial y}{\partial z}\right)_x &= 1, \\ \left(\frac{\partial z}{\partial y}\right)_x \left(\frac{\partial y}{\partial x}\right)_z \left(\frac{\partial x}{\partial z}\right)_y &= -1. \end{aligned}$$

The latter identity is often called the *cyclic chain rule*, and admits an elegant geometric interpretation. An alternative derivation is given in Section 7.4.

7.4 Interpreting Differentials

Using differentials allows algebraic operations to yield information about differentiation. Not only do we know that

$$du = \frac{\partial u}{\partial v}\,dv + \frac{\partial u}{\partial w}\,dw \tag{7.4.1}$$

but we can also run this argument in reverse.

Suppose we know that

$$du = A\,dv + B\,dw. \tag{7.4.2}$$

where A and B may be complicated algebraic expressions involving u, v, and w. Then, by comparing Equation (7.4.1) and Equation (7.4.2), we see that

$$A = \frac{\partial u}{\partial v},$$
$$B = \frac{\partial u}{\partial w}.$$

We call this process "interpreting the partial derivatives."

Furthermore, we can use algebra to solve for dv, obtaining

$$dv = \frac{1}{A}\,du - \frac{B}{A}\,dw, \tag{7.4.3}$$

and we can conclude that

$$\left(\frac{\partial v}{\partial u}\right)_w = \frac{1}{A},$$
$$\left(\frac{\partial v}{\partial w}\right)_u = -\frac{B}{A}.$$

With so many variables in use at the same time, it became important to specify which ones are being held constant when taking derivatives; this is done by writing $\left(\frac{\partial v}{\partial u}\right)_w$ to denote the partial derivative of v with respect to u "with w held constant." We have therefore shown that

$$\left(\frac{\partial u}{\partial v}\right)_w \left(\frac{\partial v}{\partial u}\right)_w = 1,$$
$$\left(\frac{\partial u}{\partial v}\right)_w \left(\frac{\partial v}{\partial w}\right)_u + \left(\frac{\partial u}{\partial w}\right)_v = 0,$$

and the latter of these equations is usually rewritten in the form

$$\left(\frac{\partial u}{\partial v}\right)_w \left(\frac{\partial v}{\partial w}\right)_u \left(\frac{\partial w}{\partial u}\right)_v = -1 \tag{7.4.4}$$

and called the *cyclic chain rule*.

In practice, using algebra to rearrange equations involving differentials automatically incorporates the chain rule in all of these forms. It is often easier to rearrange and interpret than to use the formulas.

7.5 Things not to do with Differentials

Differentials are a wonderful tool for manipulating derivatives. However, it is important to remember that differentials themselves always refer to the *total*

change in a quantity. Ratios of differentials can often be interpreted as ordinary derivatives, but not as partial derivatives. Put differently, correct statements about differentials can be obtained by pulling apart an *ordinary* derivative, but never by pulling apart a *partial* derivative.

For instance, it is fine to convert the chain rule statement

$$\frac{df}{dt} = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial y}\frac{dy}{dt} \tag{7.5.1}$$

to the statement

$$df = \frac{\partial f}{\partial x}\,dx + \frac{\partial f}{\partial y}\,dy \tag{7.5.2}$$

by "multiplying" both sides by dt. In fact, we like to start with (7.5.2) and obtain the usual chain rule statement (7.5.1) by "dividing" both sides by dt. However, this can not be done with partial derivatives.

Consider for example the partial differential equation

$$\frac{\partial u}{\partial x} = x\frac{\partial u}{\partial y} \tag{7.5.3}$$

One way to obtain a solution of (7.5.3) is by separation of variables. In the absence of boundary conditions, this approach would yield a general solution of the form

$$u = \int A(c)\, e^{c(y+\frac{1}{2}x^2)}\, dc$$

in agreement with the "obvious" solution $u = f(y + \frac{1}{2}x^2)$ (which is however not in general separable):

$$\begin{aligned} & u(x,y) = X(x)Y(y) \\ \Longrightarrow\quad & \frac{1}{xX}\frac{dX}{dx} = \text{constant} = \frac{1}{Y}\frac{dY}{dy} \\ \Longrightarrow\quad & \frac{dX}{X} = cx\,dx \qquad \text{and} \qquad \frac{dY}{Y} = c\,dy \\ \Longrightarrow\quad & u = A\,e^{c(y+\frac{1}{2}x^2)}. \end{aligned}$$

Contrast this correct use of differentials with the following, incorrect, argument. Rewrite (7.5.3) as

$$du\,dy = x\,du\,dx \tag{7.5.4}$$

Now cancel du from both sides, obtaining

$$dy = x\,dx \tag{7.5.5}$$

suggesting that the "solution" to (7.5.3) is given by

$$y = \frac{1}{2}x^2. \tag{7.5.6}$$

The moral is that *partial* derivatives can not be treated as ratios of differentials. Do not be misled by (7.5.2) itself, which does indeed imply that

$$df = \frac{\partial f}{\partial x}\,dx \tag{7.5.7}$$

if $y =$ constant; that assumption effectively turns the partial derivative into an ordinary derivative. If several variables are changing, "shortcuts" such as (7.5.7) are not valid.

Chapter 8

The Vector Differential

8.1 The Vector Differential $d\vec{\boldsymbol{r}}$

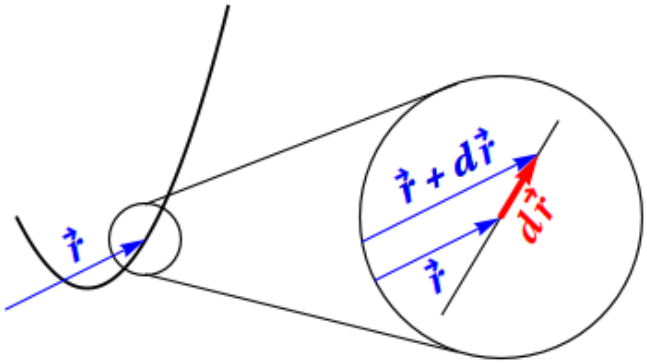


Figure 8.1.1 The infinitesimal displacement vector $d\vec{\boldsymbol{r}}$ along a curve, shown in an "infinite magnifying glass". In this and subsequent figures, artistic license has been taken in the overall scale and the location of the origin in order to make a pedagogical point.

The *position vector*

$$\vec{\boldsymbol{r}} = x\,\hat{\boldsymbol{x}} + y\,\hat{\boldsymbol{y}} + z\,\hat{\boldsymbol{z}} \tag{8.1.1}$$

describes the location of the point (x, y, z) in rectangular coordinates, and is usually thought of as pointing from the origin to that point. It is instructive to draw a picture of the small change $\Delta\vec{\boldsymbol{r}} = \Delta x\,\hat{\boldsymbol{x}} + \Delta y\,\hat{\boldsymbol{y}} + \Delta z\,\hat{\boldsymbol{z}}$ in the position vector between nearby points. Try it! This picture is so useful that we will go one step further, and consider an *infinitesimal* change in position. Instead of $\Delta\vec{\boldsymbol{r}}$, we will write $d\vec{\boldsymbol{r}}$ for the vector between two points which are infinitesimally close together. This is illustrated in Figure 8.1.1, which shows a view of the curve through an "infinite magnifying glass".

Like any vector, $d\vec{\boldsymbol{r}}$ can be expanded with respect to $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, $\hat{\boldsymbol{z}}$; the components of $d\vec{\boldsymbol{r}}$ are just the infinitesimal changes dx, dy, dz, in the x, y, and z directions, respectively, that is

$$d\vec{\boldsymbol{r}} = dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}} \tag{8.1.2}$$

as shown in Figure 8.1.2, The geometric notion of $d\vec{\boldsymbol{r}}$ as an infinitesimal vector displacement will be a unifying theme to help us in visualizing the geometry of all of vector calculus.

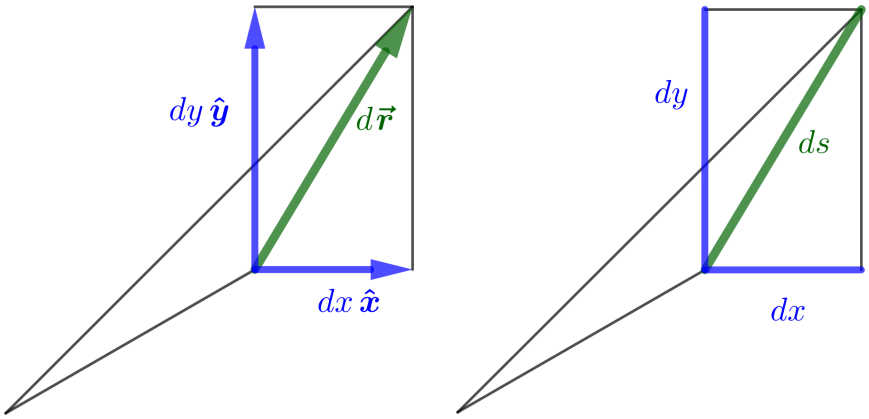


Figure 8.1.2 The first figure shows the rectangular components of the vector differential $d\vec{\boldsymbol{r}}$ in two dimensions, while the second figure shows the infinitesimal version of the Pythagorean Theorem.

What is the infinitesimal distance ds between nearby points? Just the length of $d\vec{\boldsymbol{r}}$. We have

$$ds = |d\vec{\boldsymbol{r}}| = \sqrt{d\vec{\boldsymbol{r}} \cdot d\vec{\boldsymbol{r}}} = \sqrt{dx^2 + dy^2 + dz^2} \tag{8.1.3}$$

and squaring both sides leads to

$$ds^2 = |d\vec{\boldsymbol{r}}|^2 = d\vec{\boldsymbol{r}} \cdot d\vec{\boldsymbol{r}} = dx^2 + dy^2 + dz^2 \tag{8.1.4}$$

which is just the infinitesimal Pythagorean Theorem, the two-dimensional version of which is shown in Figure 8.1.2. [1]

8.2 Finding $d\vec{\boldsymbol{r}}$ on Rectangular Paths

In the activity below, you will construct the vector differential $d\vec{\boldsymbol{r}}$ in rectangular coordinates. This vector differential is the building block used to construct multi-dimensional integrals, including flux, surface, and volume integrals, so long as they are expressed in rectangular coordinates.

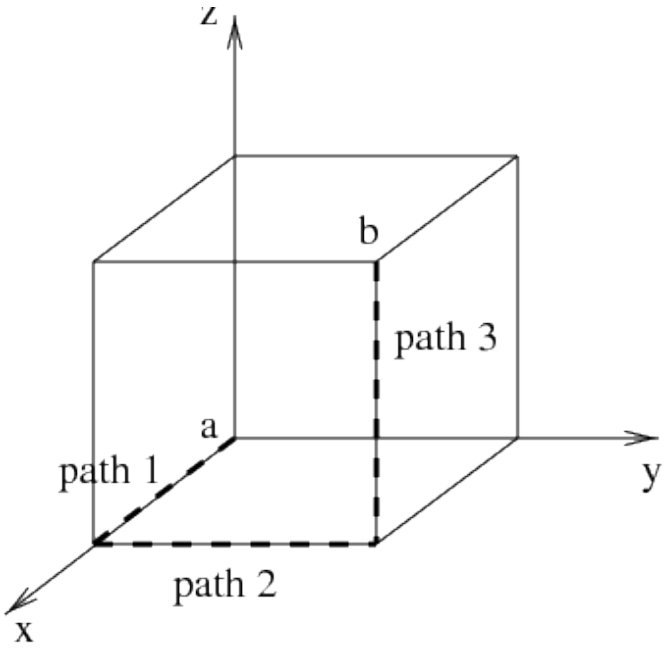
Activity 8.2.1 The Vector Differential in Rectangular Coordinates. The arbitrary infinitesimal displacement vector in Cartesian coordinates is:

$$d\vec{\boldsymbol{r}} = dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}} \tag{8.2.1}$$

Given the cube shown below, find $d\vec{\boldsymbol{r}}$ on each of the three paths, leading from a to b. Notice that the vector differential in Equation (8.2.1) has both a magnitude and a direction.

Path 1: $d\vec{\boldsymbol{r}} =$
Path 2: $d\vec{\boldsymbol{r}} =$
Path 3: $d\vec{\boldsymbol{r}} =$

[1] When dealing with infinitesimals, we prefer to avoid second-order errors by anchoring all vectors to the same point.



8.3 Other Coordinate Systems

It is important to realize that $d\vec{\boldsymbol{r}}$ and ds are defined geometrically, not by the component expressions in (8.1.2) and (8.1.4). Because of this coordinate-independent nature of $d\vec{\boldsymbol{r}}$, it is possible and useful to study $d\vec{\boldsymbol{r}}$ in another coordinate system, such as polar coordinates (r,ϕ) in the plane.[1] It is then natural to use basis vectors $\{\hat{\boldsymbol{r}}, \hat{\boldsymbol{\phi}}\}$ adapted to these coordinates, with $\hat{\boldsymbol{r}}$ being the unit vector in the radial direction, and $\hat{\boldsymbol{\phi}}$ being the unit vector in the direction of increasing ϕ; see Section 1.12. [2]

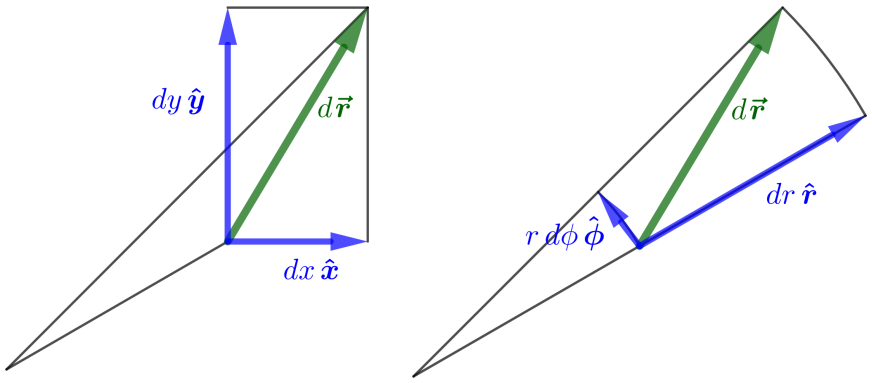


Figure 8.3.1 The infinitesimal vector version of the Pythagorean Theorem, in both rectangular and polar coordinates.

By determining the lengths of the sides of the infinitesimal polar "rectangle" shown in the last drawing of Figure 8.3.1, one obtains

$$d\vec{\boldsymbol{r}} = dr\,\hat{\boldsymbol{r}} + r\,d\phi\,\hat{\boldsymbol{\phi}} \tag{8.3.1}$$

[1] We choose ϕ for the polar angle in order to agree with the standard conventions for spherical coordinates used by everyone but (American) mathematicians.

[2] One can of course relate $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{\phi}}$ to $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$, for instance using the second figure in Figure 1.20.1. However, in most physical applications (as opposed to problems in calculus textbooks) this step can be avoided by making an appropriate initial choice of coordinates.

Notice the factor of r in the $\hat{\boldsymbol{\phi}}$ term; $d\phi$ by itself is not a *length*. The length of an infinitesimal arc is $r\,d\phi$. Using (8.1.3) to find the length of $d\vec{\boldsymbol{r}}$ as before leads to

$$ds^2 = dr^2 + r^2\,d\phi^2 \tag{8.3.2}$$

which is the infinitesimal Pythagorean Theorem in polar coordinates.

8.4 Calculating Infinitesimal Distance in Cylindrical and Spherical Coordinates

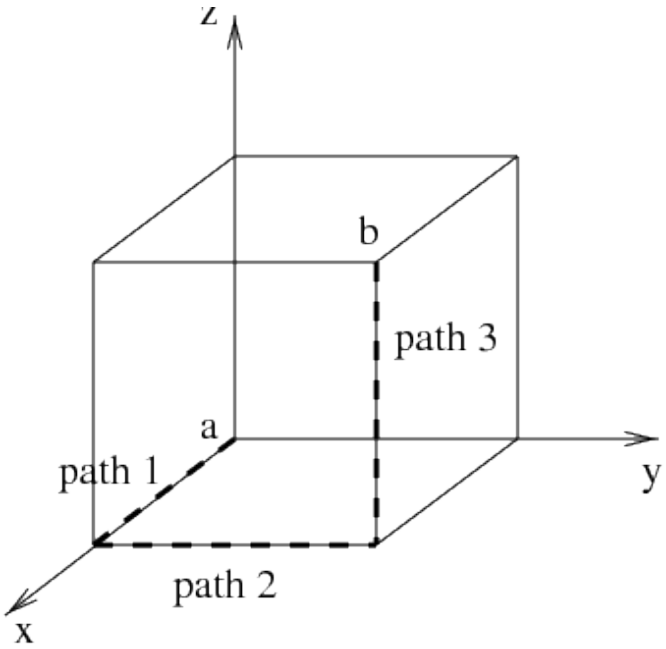
In the activities below, you will construct infinitesimal distance elements (sometimes called line elements) in rectangular, cylindrical, and spherical coordinates. These infinitesimal distance elements are building blocks used to construct multi-dimensional integrals, including surface and volume integrals. To construct flux integrals, you will need vector differentials, which are a slight variant of the infinitesimal distance elements. See Section 8.5.

Activity 8.4.1 The Distance Element in Rectangular Coordinates. Given the cube shown below, find ds on each of the three paths, leading from a to b.

Path 1: $ds =$

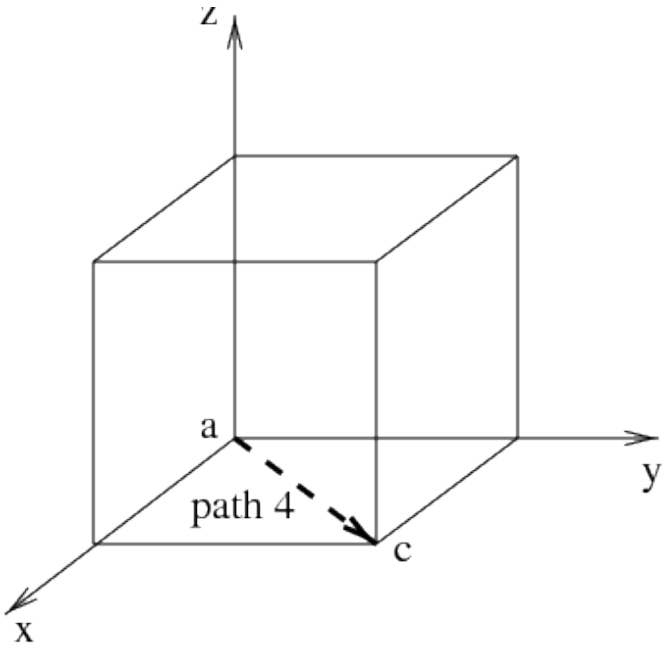
Path 2: $ds =$

Path 3: $ds =$



The infinitesimal distance element ds is an infinitesimal *length*. Find the appropriate expression for ds for the path which goes directly from a to c as drawn below.

Path 4: $ds =$



Hint. An infinitesimal element of length in the z-direction is simply dz

Cartesian coordinates would be a *poor* choice to describe a path on a cylindrically or spherically shaped surface. Next we will find appropriate expressions in these cases.

Activity 8.4.2 The Distance Element in Cylindrical Coordinates.

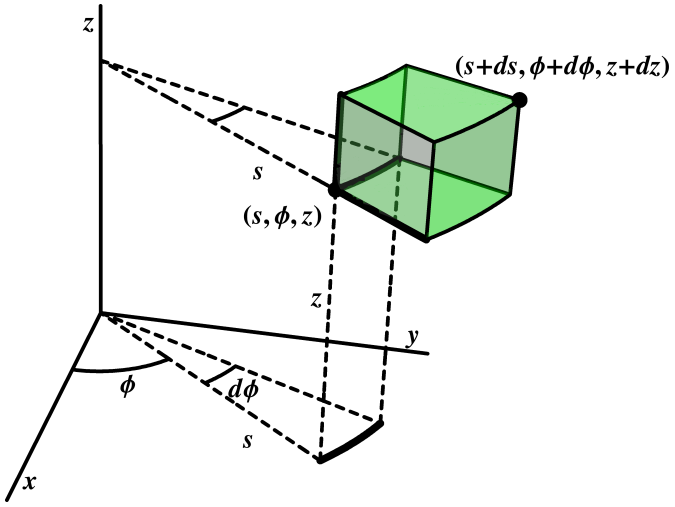


Figure 8.4.1 An infinitesimal box in cylindrical coordinates

You will now use geometry to determine the general form for ds in cylindrical coordinates by determining ds along the specific paths below. See Figure 8.4.1.

Geometrically determine the length of the three paths leading from a to b. Notice that, along any of these three paths, only one coordinate s, ϕ, or z is changing at a time (i.e. along path 1, $dz \neq 0$, but $d\phi = 0$ and $dr = 0$).

Path 1: $ds =$

Path 2: $ds =$

Path 3: $ds =$

If all three coordinates are allowed to change simultaneously, by an infinites-

imal amount, we could write this ds for any path as:

$ds=$

This is the general distance element in cylindrical coordinates.

Hint. Analogously to rectangular coordinates, an infinitesimal element of length in the r direction is simply dr. But an infinitesimal element of length in the ϕ direction in cylindrical coordinates is *not* just $d\phi$, since this would be an angle and does not even have the units of length.

Using the relationship between angles (in radians!) and radius, the infinitesimal element of length in the ϕ direction in cylindrical coordinates is $s\,d\phi$.

Activity 8.4.3 The Distance Element in Spherical Coordinates.

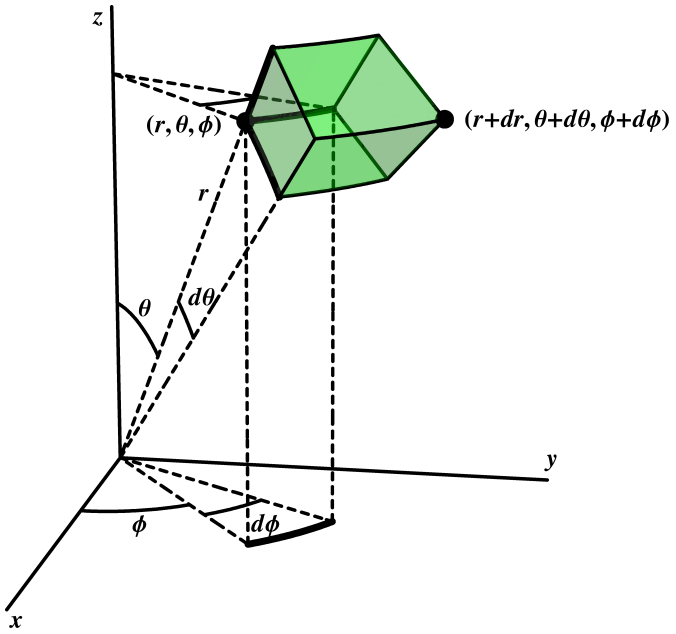


Figure 8.4.2 An infinitesimal box in spherical coordinates

You will now use geometry to determine the general form for ds in spherical coordinates by determining ds along the specific paths below. See Figure 8.4.2. As in the cylindrical case, note that an infinitesimal element of length in the $\hat{\boldsymbol{\theta}}$ or $\hat{\boldsymbol{\phi}}$ direction is *not* just $d\theta$ or $d\phi$. You will need to be more careful.

Geometrically determine the length of the three paths leading from a to b. Notice that, along any of these three paths, only one coordinate r, θ, or ϕ is changing at a time (i.e. along path 1, $d\theta \neq 0$, but $dr = 0$ and $d\phi = 0$).

Path 1: $ds =$

Path 2: $ds =$ (Be careful, this is the tricky one.)

Path 3: $ds =$

If all 3 coordinates are allowed to change simultaneously, by an infinitesimal amount, we could write this ds for any path as:

$ds=$

This is the general line element in spherical coordinates.

Hint. A similar argument to the one used above for cylindrical coordinates, shows that the infinitesimal element of length in the θ direction in spherical coordinates is $r\,d\theta$.

What about the infinitesimal element of length in the ϕ direction in spherical coordinates? Make sure to study the diagram carefully. Where is the center of a circle of constant latitude? It is *not* at the center of the sphere, but rather along the z-axis. The radius of this circle is not r, but rather $r\sin\theta$, so the

infinitesimal element of length in the ϕ direction in spherical coordinates is $r \sin\theta \, d\phi$.

8.5 Calculating $d\vec{r}$ in Curvilinear Coordinates

In Section 8.2, you discovered how to write $d\vec{r}$ in rectangular coordinates. However, this coordinate system would be a *poor* choice to describe a path on a cylindrically or spherically shaped surface. We will now find appropriate expressions in these cases.

Activity 8.5.1 The Vector Differential in Cylindrical Coordinates.

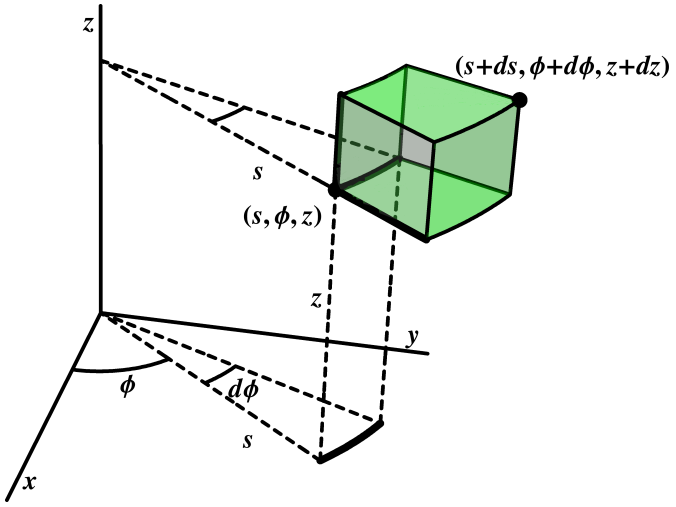


Figure 8.5.1 An infinitesimal box in cylindrical coordinates

You will now use geometry to determine the general form for $d\vec{r}$ in cylindrical coordinates by determining $d\vec{r}$ along the specific paths below. See Figure 8.5.1.

Note that an infinitesimal element of length in the $\hat{\boldsymbol{s}}$ direction is simply ds, just as an infinitesimal element of length in the $\hat{\boldsymbol{x}}$ direction is dx. *But*, an infinitesimal element of length in the $\hat{\boldsymbol{\phi}}$ direction is *not* just $d\phi$, since this would be an angle and does not have the units of length.

Geometrically determine the length of the three paths leading from a to b and write these lengths in the corresponding boxes on the diagram.

Now, remembering that $d\vec{r}$ has both magnitude and direction, write the infinitesimal displacement vector $d\vec{r}$ along the three bold paths from the point (s, ϕ, z) to b. Notice that, along any of these three paths, only one coordinate s, ϕ, or z is changing at a time (i.e. along path 1, $dz \neq 0$, but $d\phi = 0$ and $ds = 0$).

Path 1: $d\vec{r} =$

Path 2: $d\vec{r} =$

Path 3: $d\vec{r} =$

If all three coordinates are allowed to change simultaneously, by an infinitesimal amount, we could write this $d\vec{r}$ for any path as:

$d\vec{r}=$

This is the general line element in cylindrical coordinates.

Hint. Make sure you think about what the correct lengths are in each coordinate direction. Angles are not lengths!

Solution. Upon completing this activity, you should have obtained the expressions

$$d\vec{r} = dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}}$$

$$= ds\,\hat{\boldsymbol{s}} + s\,d\phi\,\hat{\boldsymbol{\phi}} + dz\,\hat{\boldsymbol{z}}$$

in rectangular and cylindrical coordinates, respectively.

Activity 8.5.2 The Vector Differential in Spherical Coordinates.

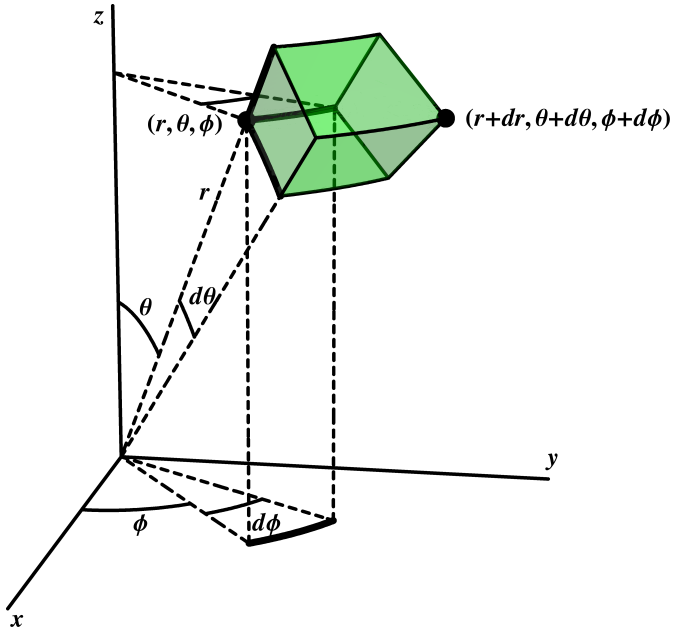


Figure 8.5.2 An infinitesimal box in spherical coordinates

You will now use geometry to determine the general form for $d\vec{\boldsymbol{r}}$ in spherical coordinates by determining $d\vec{\boldsymbol{r}}$ along the specific paths below. See Figure 8.5.2. As in the cylindrical case, note that an infinitesimal element of length in the $\hat{\boldsymbol{\theta}}$ or $\hat{\boldsymbol{\phi}}$ direction is *not* just $d\theta$ or $d\phi$. You will need to be more careful. Geometrically determine the length of the three bold paths leading from (r, θ, ϕ) and write these lengths below. Now, remembering that $d\vec{\boldsymbol{r}}$ has both magnitude and direction, write down below the infinitesimal displacement vector $d\vec{\boldsymbol{r}}$ along the three paths. Notice that, along any of these three paths, only one coordinate r, θ, or ϕ is changing at a time (i.e. along path 1, $d\theta \neq 0$, but $dr = 0$ and $d\phi = 0$).

Path 1: $d\vec{\boldsymbol{r}} =$

Path 2: $d\vec{\boldsymbol{r}} =$ (Be careful, this is the tricky one.)

Path 3: $d\vec{\boldsymbol{r}} =$

If all three coordinates are allowed to change simultaneously, by an infinitesimal amount, we could write this $d\vec{\boldsymbol{r}}$ for any path as:

$d\vec{\boldsymbol{r}}=$

This is the general line element in spherical coordinates.

Hint. As before, make sure you think about what the correct lengths are in each coordinate direction, and recall that angles are not lengths. Also make sure you know the radius of a circle of constant latitude.

Solution. Upon completing the worksheet, you should have obtained the expressions

$$\begin{aligned} d\vec{\boldsymbol{r}} &= dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}} \\ &= ds\,\hat{\boldsymbol{s}} + s\,d\phi\,\hat{\boldsymbol{\phi}} + dz\,\hat{\boldsymbol{z}} \\ &= dr\,\hat{\boldsymbol{r}} + r\,d\theta\,\hat{\boldsymbol{\theta}} + r\,\sin\theta\,d\phi\,\hat{\boldsymbol{\phi}} \end{aligned}$$

in rectangular, cylindrical, and spherical coordinates, respectively.

8.6 Scalar Surface Elements

Activity 8.6.1 Scalar Surface Elements. Using the expressions for the infinitesimal elements of length derived and discussed in Sections 8.4 and Section 8.4, you should find explicit formulas for the surface or volume elements in each of the following cases:

- the scalar surface elements for the three surfaces (top, bottom, and curved side) of a cylinder with finite length;
- the scalar surface element for a horizontal plane through the z-axis;
- the scalar surface element for the surface of a sphere.
- the volume element of a cylinder;
- the volume element for a sphere.

You may find the diagrams in Section 8.4 to be helpful.

Hint. Evaluating surface integrals in other coordinate systems involves the same idea as double integrals in rectangular coordiantes: chop and add. The difference is in the way one chops.

Solution. In polar coordinates, one chops a region into pie shaped regions using radial lines and circles. These lines are orthogonal to each other, so that a small enough piece is nearly rectangular, which means that its area is just its length times its width. As discussed in [1], a little thought shows that a radial side has length ds, but a circular side has length $s\,d\phi$ — not merely $d\phi$, which has the wrong units. Thus, in polar coordinates,

$$dA = s\,ds\,d\phi \tag{8.6.1}$$

The same argument shows that a small piece of the surface of a cylinder has area given by

$$dA = s\,d\phi\,dz \tag{8.6.2}$$

since the two sides of the rectangle have lengths $s\,d\phi$ and dz. This construction is illustrated in Figure 8.4.1 (which can also be used for polar coordinates if one ignores the vertical path).

Spherical coordinates can be handled similarly. The two sides are parts of lines of longitude and latitude. Segments along lines of longitude ("vertical") have length $r\,d\theta$, but segments along lines of latitude ("horizontal") have length $r\sin\theta\,d\phi$ — the radius of the circle depends on the latitude, hence the extra factor, which turns out to be $\sin\theta$. Thus, on the surface of a sphere we have

$$dA = r^2\sin\theta\,d\theta\,d\phi \tag{8.6.3}$$

This construction is illustrated in Figure 8.4.2.

Similar arguments apply to triple integrals, as discussed in Section 8.7.

8.7 Triple Integrals in Cylindrical and Spherical Coordinates

Evaluating multiple integrals in other coordinate systems involves the same idea as in rectangular coordinates: chop and add. The difference is in the way one chops.

In cylindrical coordinates, one chops a region into small pieces that look like "pineapple chunks", with volume dV (or $d\tau$ in another common notation) given by

$$dV = s\,ds\,d\phi\,dz. \tag{8.7.1}$$

This construction is illustrated in Figure 8.4.1 (which can also be used for polar coordinates if one ignores the vertical path).

Spherical coordinates can be handled similarly, where the small pieces now look like parts of orange segments. The radial side still has length dr, and the other two sides can be thought of as (parts of) lines of longitude and latitude. Segments along lines of longitude ("vertical") have length $r\,d\theta$, but segments along lines of latitude ("horizontal") have length $r\sin\theta\,d\phi$ — the radius of the circle depends on the latitude, hence the extra factor, which turns out to be $\sin\theta$. Thus, in spherical coordinates we have

$$dV = r^2\sin\theta\,dr\,d\theta\,d\phi. \tag{8.7.2}$$

This construction is illustrated in Figure 8.4.2.

8.8 Using $d\vec{r}$ on More General Paths

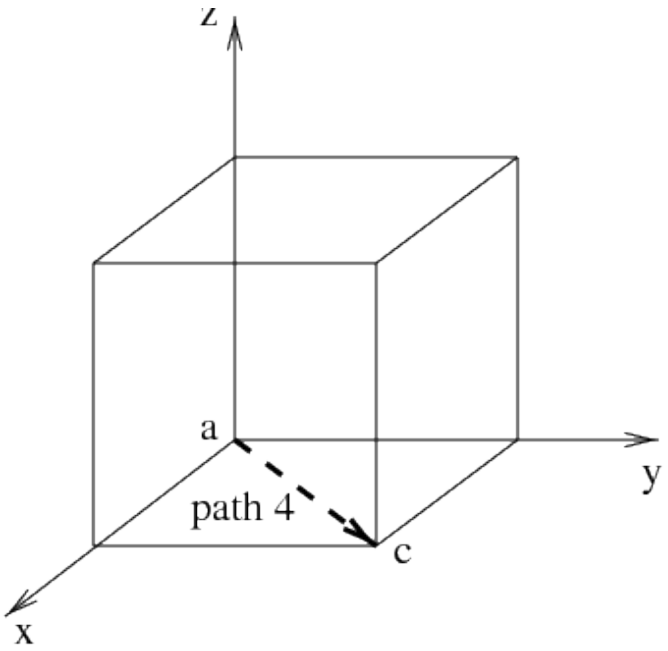
In this section, we use the formula $d\vec{r} = dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}}$ in rectangular coordinates to calculate some simple geometric/physical quantities.

Activity 8.8.1 The Vector Differential in Rectangular Coordinates. The arbitrary infinitesimal displacement vector in Cartesian coordinates is:

$$d\vec{r} = dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}} \tag{8.8.1}$$

Given the unit cube shown below, find $d\vec{r}$ on path 4, leading from a to c. Then, use this expression to find the length of the line segment between a and c.

Path 4: $d\vec{r} =$



Hint. "Use what you know!" What is the value of z on this path? How is x related to y? How is dx related to dy?

Solution. What we know on this path is that $z = 0$ and therefore $dz = 0$. We also know that $x = y$ and therefore $dx = dy$. We can plug this information into Equation (8.8.1), choosing to keep our calculations either in terms of the variable x or in terms of the variable y, but not both.

$$\begin{aligned} d\vec{\boldsymbol{r}} &= dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}} \\ &= dx\,(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}) \\ \Rightarrow |d\vec{\boldsymbol{r}}| &= |dx\,(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})| \\ &= dx\,\sqrt{(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}) \cdot (\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})} \\ &= \sqrt{2} \end{aligned}$$

Notice how using $d\vec{\boldsymbol{r}}$ automatically generates the geometric factor of $\sqrt{2}$.

We can integrate $|d\vec{\boldsymbol{r}}|$ to get the length of the line segment. Since we have expressed $|d\vec{\boldsymbol{r}}|$ in terms of dx, we must be careful to be consistent and express the limits of integration also in terms of x, i.e. for a unit cube, $0 \le x \le 1$. Be careful to integrate in a direction so that $|dx|$ is a positive direction.

$$\begin{aligned} LENGTH &= \int |d\vec{\boldsymbol{r}}| \\ &= \sqrt{2}\,|dx| \\ &= \sqrt{2}\,dx \end{aligned}$$

8.9 Use What You Know

Suppose you want to find the work done by the force $\vec{\boldsymbol{F}} = y^2\,\hat{\boldsymbol{x}} + y\,\hat{\boldsymbol{y}}$ when moving along a given curve C. Curves can be specified in several different ways; let us consider some examples, all of which refer to the same curve, starting at $(1, 0)$ and ending at $(0, 1)$.

1. Consider first the parametric curve $\vec{\boldsymbol{r}} = (1 - u^2)\,\hat{\boldsymbol{x}} + u\,\hat{\boldsymbol{y}}$. It is straightforward to compute
$$d\vec{\boldsymbol{r}} = (-2u\,\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})\,du.$$
Since a curve is described by a single parameter, in this case u, we write everything in terms of that parameter. Since $\vec{\boldsymbol{r}} = x\,\hat{\boldsymbol{x}} + y\,\hat{\boldsymbol{y}}$, we have $x = 1 - u^2$, $y = u$, and therefore
$$\begin{aligned} \int_C \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{r}} &= \int_0^1 \left(u^2\,\hat{\boldsymbol{x}} + u\,\hat{\boldsymbol{y}}\right) \cdot (-2u\,\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})\,du \\ &= \int_0^1 (-2u^3 + u)\,du = 0. \end{aligned}$$

2. In physical applications, one is rarely given an explicit parameterization of the curve, but rather some other description. For instance, the curve just discussed might have been defined by the equation $x = 1 - y^2$. Finding the differential of both sides of this expression yields $dx = -2y\,dy$, and substituting into (8.1.2) leads to
$$d\vec{\boldsymbol{r}} = (-2y\,\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})\,dy.$$
The computation is exactly the same as before, using y instead of u.

3. Alternatively, one can solve for y, obtaining $y = \sqrt{1-x}$, then compute dy in terms of dx, then substitute into (8.1.2), obtaining

$$d\vec{\boldsymbol{r}} = dx\,\hat{\boldsymbol{x}} - \frac{dx}{2\sqrt{1-x}}\,\hat{\boldsymbol{y}}$$

so that [1]

$$\int_C \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{r}} = \int_1^0 \left(\frac{1}{2} - x\right) dx = 0.$$

It is important to realize that all of these methods work; using what you know will always yield correct answers — eventually.

In a "use what you know" strategy, you may not be sure when to stop! A common error is to substitute for dy in terms of dx in $d\vec{\boldsymbol{r}}$, but to forget to substitute for y in terms of x in $\vec{\boldsymbol{F}}$. The rule of thumb is that you shouldn't start integrating until you have the integral in terms of a single parameter — including correctly determining the limits in terms of that parameter. Curves are one-dimensional!

Here is another example. Suppose you want to integrate $\int_C \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{r}}$, where $\vec{\boldsymbol{F}} = y\,\hat{\boldsymbol{x}}$, and C is the line segment from $(1, 0)$ to $(0, -1)$. Start with expression (8.1.2) for $d\vec{\boldsymbol{r}}$. What do you know? Well, the slope of the line segment is clearly $+1$, and its y-intercept is -1, so the equation of the line is $y = x - 1$. Taking the differential of both sides, $dy = dx$, so that $d\vec{\boldsymbol{r}} = dx\,\hat{\boldsymbol{x}} + dx\,\hat{\boldsymbol{y}}$. Finally, note that x runs from 1 to 0! Thus,

$$\begin{aligned}\int_C \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{r}} &= \int_1^0 (x-1)\,\hat{\boldsymbol{x}} \cdot (\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})\,dx \\ &= \int_1^0 (x-1)\,dx = \left(\frac{x^2}{2} - x\right)\Bigg|_1^0 = \frac{1}{2}.\end{aligned}$$

Yes, of course, this particular curve is easy to parameterize, but this is not always the case. Note also how easy it was to get the limits right, and thus get the correct sign, simply by *always* starting with expression (8.1.2) for $d\vec{\boldsymbol{r}}$, and integrating from your starting point to your final point.

This is important: Vector line integrals of the form $\int_C \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{r}}$ are *directed* integrals; the sign of the answer depends on which way you traverse the curve. You will obtain the correct sign automatically if you integrate from the beginning point to the final point, without putting in any artificial signs. As in the last example, this may result in an integral which goes from a larger value of the integration variable to a smaller one.

This sign dependence is *not* the case for line integrals with respect to arclength. Since $ds = |d\vec{\boldsymbol{r}}|$, such integrals do not depend on which way the curve is traversed. Standard examples are arclength and mass, which must be positive! Other times you may have to think about it to get the sign right; the total charge on a wire could be positive or negative. One way to keep this straight is to remember that $ds = |d\vec{\boldsymbol{r}}|$, which has an absolute value in it, which requires care with signs.

We summarize this discussion by writing

$$\int_{-C} f\,ds = +\int_C f\,ds \quad \text{but} \quad \int_{-C} \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{r}} = -\int_C \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{r}} \tag{8.9.1}$$

[1] Note that y *decreases* along the curve.

where $-C$ denotes the reversed curve. You will always get the sign right for vector line integrals if you are careful to put the limits in correctly (from starting point to ending point), whereas you may have to think about signs for the scalar line integrals.

Chapter 9

Gradient

9.1 The Geometry of Gradient

How do you compute a derivative of a quantity that depends on a single variable? By taking the ratio of small changes in the quantity to small changes in the variable. But what if the quantity depends on several variables, such as the temperature in the room? Use the same strategy — but the result will depend on which direction you go.

Suppose therefore that you are given a quantity f that depends on position in space. We could express that position in terms of rectangular coordinates (x, y, z), but let's save that for later. To find the derivative of f at a given point and in a given direction, we must first specify the point and the direction. We know how to do that!

A point in space can be described in terms of the position vector $\vec{\boldsymbol{r}}$ from the origin to the given point. And the direction is determined by considering any curve through the given point; a small change in position along the curve is, of course, described by $d\vec{\boldsymbol{r}}$.

So consider the small change df in f along the curve. As $ds = |d\vec{\boldsymbol{r}}|$ shrinks to 0, so does df; the derivative of f along the curve is the (limiting value of the) ratio of the small quantities df and ds.

Now consider computing this derivative in all possible directions. There will be one direction in which the derivative is as large as possible. We define the *gradient* of f, written $\vec{\boldsymbol{\nabla}} f$, to be the vector whose direction is the direction in which f increases the fastest, and whose magnitude is the derivative of f in that direction. This construction yields the gradient of f at a given point, and we can repeat the process at any point; the gradient of f is a vector field.

How much does f change in an arbitrary direction? Suppose we have a curve through the given point that goes in this new direction. Since derivatives are linear, the rate of change along this new curve is just the projection of $\vec{\boldsymbol{\nabla}} f$ along the curve, namely

$$\frac{df}{ds} = \vec{\boldsymbol{\nabla}} f \cdot \frac{d\vec{\boldsymbol{r}}}{|d\vec{\boldsymbol{r}}|} \tag{9.1.1}$$

where $d\vec{\boldsymbol{r}}$ and ds now refer to the new curve, and are therefore different than before. Remembering that $|d\vec{\boldsymbol{r}}| = ds$, we can rewrite this expression as

$$df = \vec{\boldsymbol{\nabla}} f \cdot d\vec{\boldsymbol{r}} \tag{9.1.2}$$

which we refer to as the *Master Formula*, and which can also be taken as the *geometric definition* of the gradient.

Recall that df represents the infinitesimal change in f when moving to a "nearby" point. What information do you need in order to know how f changes? You must know something about how f behaves, where you started, and which way you went. The Master Formula organizes this information into two geometrically different pieces, namely the gradient, containing generic information about how f changes, and the vector differential $d\vec{\boldsymbol{r}}$, containing information about the particular change in position being made.

We refer to (9.1.2) as the Master Formula, because it contains all of the information needed to determine the gradient, and does so without relying on a particular coordinate system.

9.2 The Gradient in Rectangular Coordinates

As discussed in Section 6.9, the chain rule for a function of several variables, written in terms of differentials, takes the form:

$$df = \frac{\partial f}{\partial x}\,dx + \frac{\partial f}{\partial y}\,dy + \frac{\partial f}{\partial z}\,dz. \tag{9.2.1}$$

Each term is a product of two factors, labeled by x, y, and z. This looks like a dot product. Separating out the pieces, we have

$$df = \left(\frac{\partial f}{\partial x}\,\hat{\boldsymbol{x}} + \frac{\partial f}{\partial y}\,\hat{\boldsymbol{y}} + \frac{\partial f}{\partial z}\,\hat{\boldsymbol{z}}\right) \cdot (dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}}). \tag{9.2.2}$$

The last factor is just $d\vec{\boldsymbol{r}}$, and you may recognize the first factor as the gradient of f written in rectangular coordinates. Putting this all together, this algebraic observation leads us back to (9.1.2), as further discussed in Section 9.1.

With our new interpretation of (9.1.2) as the *definition* of the gradient, the argument above shows how to determine the formula for the gradient in rectangular coordinates, namely

$$\vec{\boldsymbol{\nabla}} f = \frac{\partial f}{\partial x}\,\hat{\boldsymbol{x}} + \frac{\partial f}{\partial y}\,\hat{\boldsymbol{y}} + \frac{\partial f}{\partial z}\,\hat{\boldsymbol{z}}. \tag{9.2.3}$$

9.3 Properties of the Gradient

What does the gradient mean geometrically? Along a particular path, df tells us something about how f is changing. But the Master Formula tells us that $df = \vec{\boldsymbol{\nabla}} f \cdot d\vec{\boldsymbol{r}}$, which means that the dot product of $\vec{\boldsymbol{\nabla}} f$ with a vector tells us something about how f changes along that vector. So let $\hat{\boldsymbol{w}}$ be a unit vector, and consider

$$\vec{\boldsymbol{\nabla}} f \cdot \hat{\boldsymbol{w}} = |\vec{\boldsymbol{\nabla}} f|\,|\hat{\boldsymbol{w}}| \cos\theta = |\vec{\boldsymbol{\nabla}} f| \cos\theta \tag{9.3.1}$$

which is clearly maximized by $\theta = 0$. Thus, the *direction* of $\vec{\boldsymbol{\nabla}} f$ is just the direction in which f increases the fastest, and the *magnitude* of $\vec{\boldsymbol{\nabla}} f$ is the rate of increase of f in that direction (per unit distance, since $\hat{\boldsymbol{w}}$ is a unit vector). If you visualize the value of the scalar field f as represented by color, then the gradient points in the direction in which the rate of change of the color is greatest.

You can also visualize the gradient using the *level surfaces* on which $f(x, y, z) =$ const. (In two dimensions there is the analogous concept of *level curves*, on which $f(x, y) =$ const.) Consider a small displacement $d\vec{\boldsymbol{r}}$ that

lies on the level surface, that is, start at a point on the level surface, and move along the surface. Then f doesn't change in that direction, so $df = 0$. But then

$$0 = df = \vec{\nabla} f \cdot d\vec{r} = 0 \tag{9.3.2}$$

so that $\vec{\nabla} f$ is perpendicular to $d\vec{r}$. Since this argument works for *any* vector displacement $d\vec{r}$ in the surface, $\vec{\nabla} f$ must be perpendicular to the level surface.

If you prefer working with derivatives instead of differentials, consider a curve $\vec{r}(u)$ that lies in the level surface. Now simply divide (9.3.2) by du, obtaining

$$0 = \frac{df}{du} = \vec{\nabla} f \cdot \frac{d\vec{r}}{du} = 0 \tag{9.3.3}$$

so that $\vec{\nabla} f$ is perpendicular to the tangent vector $\frac{d\vec{r}}{du}$ (which is just the velocity vector if the parameter u represents time). Again, this argument applies to any curve in the level surface, so $\vec{\nabla} f$ must be perpendicular to every such curve. In other words, $\vec{\nabla} f$ is perpendicular to the level surfaces of f, that is

$$\vec{\nabla} f \perp \{f(x, y, z) = \text{ const}\}. \tag{9.3.4}$$

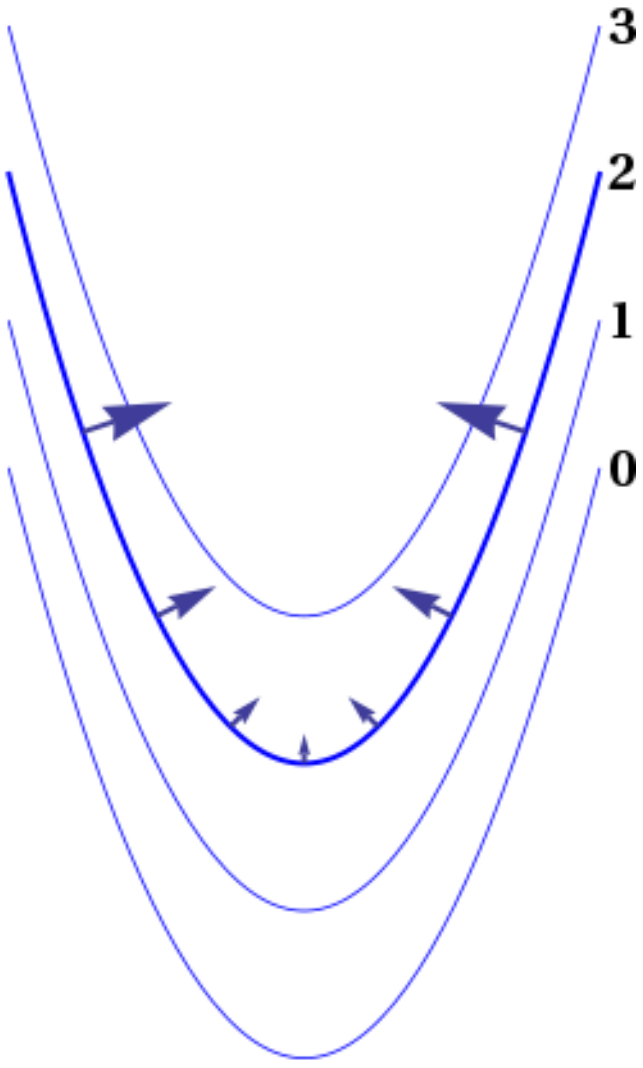


Figure 9.3.1 Gradient vectors along a level curve.

This orthogonality is shown for the case of level curves in Figure 9.3.1, which shows the gradient vector at several points along a particular level curve among several. You can think of such diagrams as *topographic maps*, showing the "height" at any location. The magnitude of the gradient vector is greatest where the level curves are close together, so that the "hill" is steepest.

An alternative way of seeing this orthogonality is to recognize that, since the gradient is a derivative operator, its value depends only on what is happening locally. If you zoom in close enough to a given point, the level surfaces are parallel, and the gradient points in the direction from one level surface to the next.

Like all derivative operators, the gradient is linear (the gradient of a sum is the sum of the gradients), and also satisfies a product rule

$$\vec{\boldsymbol{\nabla}}(fg) = (\vec{\boldsymbol{\nabla}}f)\,g + f\,(\vec{\boldsymbol{\nabla}}g). \tag{9.3.5}$$

This formula can be obtained either by working out its components in, say, rectangular coordinates, and using the product rule for partial derivatives, or directly from the product rule in differential form, which is

$$d(fg) = (df)\,g + f\,(dg) \tag{9.3.6}$$

as discussed in Section 6.5.

9.4 Visualizing the Geometry of the Gradient

The activity below is designed to help you understand the geometry of topographic maps and the gradient vector.

Activity 9.4.1 Suppose you are standing on a hill. You have a topographic map, which uses rectangular coordinates (x, y) measured in miles. Your global positioning system says your present location is at one of the following points (pick one):

$$A{:}(1,4), \quad B{:}(4-9), \quad C{:}(-4,9), \quad D{:}(1,-4), \quad E{:}(2,0), \quad F{:}(0,3).$$

Your guidebook tells you that the height h of the hill in feet above sea level is given by

$$h = a - bx^2 - cy^2$$

where $a = 5000$ ft, $b = 30\ \frac{\text{ft}}{\text{mi}^2}$, and $c = 10\ \frac{\text{ft}}{\text{mi}^2}$.

1. Where is the top of the hill located?
2. How high is the hill?
3. Draw a topographic map of the hill. *Your map should have at least 3 level curves; label your location on the map.*
4. What is your height?
5. Starting at your present location, in what map direction (2-d unit vector) do you need to go in order to climb the hill as steeply as possible? *Draw this vector on your topographic map.*
6. How steep is the hill if you start at your present location and go in this compass direction? *Draw a picture which shows the slope of the hill at your present location.*

7. In what direction in space (3-d vector) would you actually be moving if you started at your present location and walked in the map direction you found above? *To simplify the computation, your answer does* not *need to be a unit vector.*

8. Stand up and imagine yourself standing at your chosen point on the hill — you will need to decide where the top of the hill is located. Now point in the direction of the gradient at your location.

Hint.

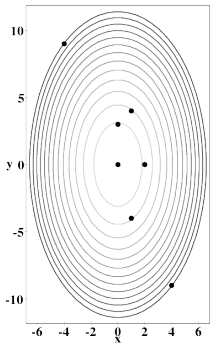


Figure 9.4.1 The topgraphic map of the hill.

Figuring out the location of the top of the hill, and its height, should have been straightforward. But drawing level curves — the topo map for the hill, shown in Figure 9.4.1 — is not so easy. Don't skip this step! Feel free to use a graphics program to generate these drawings, but it is important to develop the ability to translate between equations and topo maps.

A key feature that you should have realized while answering these questions is that the gradient lives in the topo map, not on the hill. Although we think of the gradient as pointing "uphill", the gradient of a function of two variables is a vector in the xy-plane. In particular, when answering the last question, your hand should have been horizontal!

In order to find the 3-dimensional vector direction of travel, you will need to combine a horizontal vector in the direction of the gradient with a vertical vector scaled so that the ratio is the steepness of the hill at the given point — which is given by the magnitude of the gradient. It is probably easiest, but not necessary, to choose the horizontal part of this vector to be a unit vector. Make sure you get the units right!

A possible extension would be to answer the same questions for the hill given by

$$h = 2xy - 3x^2 - 4y^2 - 18x + 28y + 1200.$$

9.5 Using Technology to Visualize the Gradient

The gradient of a function of three variables is a vector at each point in space. How can we graph such vector fields? How many different ways can you represent this information?

Activity 9.5.1 Using technology to visualize the gradient. After you have thought about these questions yourself, you can use the Sage code below

to explore several different mechanisms for visualizing the gradient in two and three dimensions. You can also use this Mathematica notebook[1] for the same purpose.

The code in the first box does some initialization, then defines and plots a function of two variables.

```
pretty_print_default(True)
from sage.manifolds.operators import *
E.<x,y>=EuclideanSpace()
E.default_frame()[1].set_name(latex_name=r'\,\boldsymbol{\hat{x}}')
E.default_frame()[2].set_name(latex_name=r'\,\boldsymbol{\hat{y}}')
f(x,y)=exp(-x^2)*exp(-y^2)
p3=plot3d(f(x,y),(x,-1,1),(y,-1,1),adaptive=true)
p3
```

Now we can plot a contour diagram of the chosen function f.

```
pc=contour_plot(f(x,y),(x,-1,1),(y,-1,1),linewidths=0)
pc
```

Next we compute the gradient of f...

```
gf=f.gradient()
# gf(x,y)
E.vector_field(gf).display()
```

... and plot it. [2]

```
pg=plot_vector_field(gf,(x,-1,1),(y,-1,1),plot_points=11)
pg
```

Finally, we display both plots together. What do you notice?

```
pc+pg
```

Now try other functions by plugging something else in for $f(x, y)$ in the first box and then redoing the other steps. A particularly nice choice is $f = e^{y^2-x^2}$.

Hint.

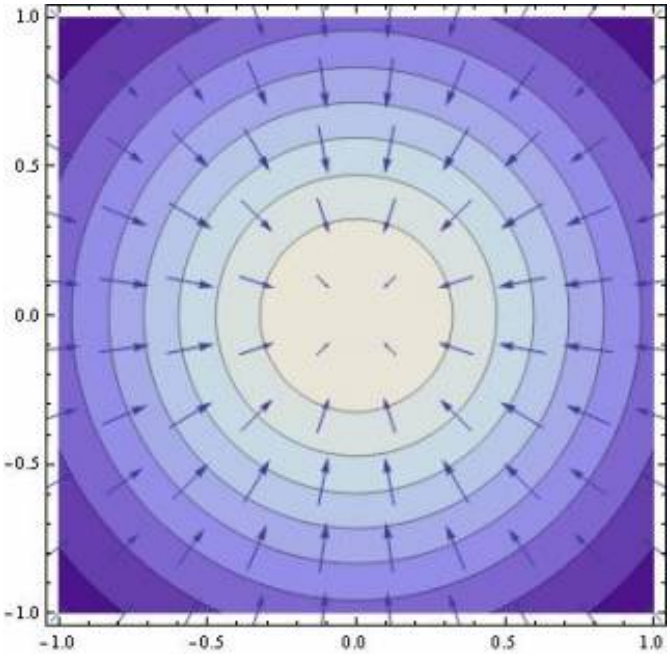


Figure 9.5.1 The gradient in 2 dimensions.

In the activity in Section 9.5, you were asked to explore different ways of representing the gradient graphically. One combined representation is shown in Figure 9.5.1, showing both the gradient vector field and the level curves.

9.6 Contour Diagrams

Figure 9.6.1 shows the relationship between tables of data, contour lines, and contour diagrams. Figure 9.6.2 then shows the relationship of contour diagrams to the underlying graph.

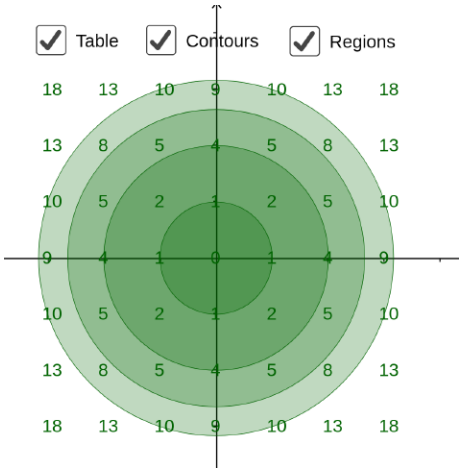


Figure 9.6.1 The relationship between tables of data and contour diagrams. Click on the check boxes to examine each of these features separately.

[1] `math.oregonstate.edu/bridge/paradigms/vfgradient.nb`

[2] You may need to adjust the value of the scale option in this plot, which controls the overall scale of the vectors drawn.

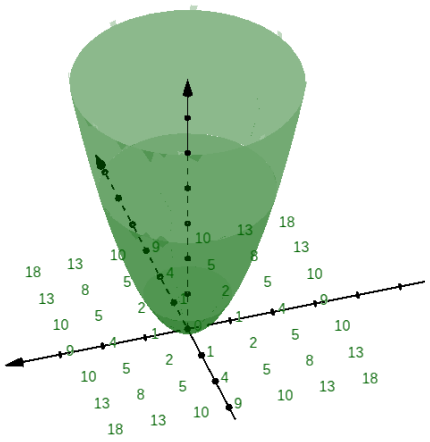


Figure 9.6.2 The relationship between contour diagrams and graphs. Click and drag the figure!

Activity 9.6.1 Can you determine the function whose data is shown in Figures 9.6.1–9.6.2?

Solution. The level sets are circles, each with an equation of the form $x^2+y^2 =$ constant. So the underlying function is $f(x, y) = x^2+y^2$. The three-dimensional graph (click and drag!) in Figure 9.6.2 shows the paraboloid $z = x^2 + y^2$, that is, $z = f(x, y)$.

Activity 9.6.2 Using technology to visualize level sets. After you have thought about these questions yourself, you can use the Sage code below to explore several different mechanisms for visualizing level sets in two dimensions. The code in the first box defines and plots a function of two variables.

```
f(x,y)=exp(-x^2)*exp(-y^2)
p3=plot3d(f(x,y),(x,-1,1),(y,-1,1),adaptive=true)
p3
```

Now we can plot a contour diagram of the chosen function f.

```
pc=contour_plot(f(x,y),(x,-1,1),(y,-1,1),linewidths=0)
pc
```

Now try other functions by plugging something else in for $f(x, y)$ in the first box and then redoing the other steps. A particularly nice choice is $f = e^{y^2-x^2}$.

9.7 Directional Derivatives

Differentials such as *df* are rarely themselves the answer to any physical question. So what good is the Master Formula? The short answer is that you can use it to answer *any* question about how f changes. Here are some examples.

- *Suppose you are an ant walking in a puddle on a flat table. The depth of the puddle is given by $h(x, y)$. You are given x and y as functions of time t. How fast is the depth of water through which you are walking changing per unit time?*

This problem is asking for the derivative of h with respect to t. So divide the Master Formula by dt to get

$$\frac{dh}{dt} = \vec{\boldsymbol{\nabla}} h \cdot \frac{d\vec{\boldsymbol{r}}}{dt}$$

where $\vec{\boldsymbol{r}}$ describes the particular path you are taking. The factor $\frac{d\vec{\boldsymbol{r}}}{dt}$ is simply your velocity. This dot product is easy to evaluate, and yields the answer to the question.

(There are of course many ways to solve this problem; which method you choose may depend on how your path is described. It is often easiest to simply insert the given expressions for x and y in terms of t directly into h, then differentiate the resulting function of a single variable, thus calculating the left-hand side directly.)

- *You are another ant on the same surface, moving on a path with $y = 3x$. How fast is the depth changing compared with x?*

This problem is asking for the derivative of h with respect to x *as you move along the path*; note that this is the total derivative $\frac{dh}{dx}$, not the partial derivative $\frac{\partial h}{\partial x}$, which would only be appropriate if y were constant along the path. So divide the Master Formula by dx to get

$$\frac{dh}{dx} = \vec{\boldsymbol{\nabla}} h \cdot \frac{d\vec{\boldsymbol{r}}}{dx}$$

then use what you know ($y = 3x$) to relate the changes in x and y ($dy = 3\,dx$), so that

$$d\vec{\boldsymbol{r}} = dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} = dx\,\hat{\boldsymbol{x}} + 3\,dx\,\hat{\boldsymbol{y}} = (\hat{\boldsymbol{x}} + 3\,\hat{\boldsymbol{y}})\,dx$$

to obtain

$$\frac{d\vec{\boldsymbol{r}}}{dx} = \hat{\boldsymbol{x}} + 3\,\hat{\boldsymbol{y}}.$$

Evaluating the dot product yields the answer to the question.

- *You are still moving on the same surface, but now the question is, how fast is the depth changing per unit distance along the path?*

This problem is asking for the derivative of h with respect to arclength ds. We can divide the Master Formula by ds, which leads to

$$\frac{dh}{ds} = \vec{\boldsymbol{\nabla}} h \cdot \frac{d\vec{\boldsymbol{r}}}{ds}.$$

Unfortunately, it is often difficult to determine s; it is not always possible to express h as a function of s. On the other hand, all we need to know is that

$$ds = |d\vec{\boldsymbol{r}}|$$

so that dividing $d\vec{\boldsymbol{r}}$ by ds is just dividing by its length; the result must be a unit vector! Which unit vector? The one tangent to your path, namely the unit tangent vector $\hat{\boldsymbol{T}}$, so

$$\frac{dh}{ds} = \vec{\boldsymbol{\nabla}} h \cdot \hat{\boldsymbol{T}}. \tag{9.7.1}$$

Evaluating the dot product answers the question, without ever worrying about arclength.

We have just seen that the derivative of f along a curve splits into two parts: a derivative of f (namely $\vec{\boldsymbol{\nabla}} f$), and a derivative of the curve ($d\vec{\boldsymbol{r}}/du$).

But the latter depends only on the tangent direction of the curve at the given point, not on the detailed shape of the curve. This leads us to the concept of the *directional derivative* of f at a particular point $\vec{\boldsymbol{r}} = \vec{\boldsymbol{r}}_0 = \vec{\boldsymbol{r}}(u_0)$ *along* the vector $\vec{\boldsymbol{v}}$, which is traditionally defined as follows: [1]

$$D_{\vec{\boldsymbol{v}}} f = \lim_{\epsilon \to 0} \frac{f(\vec{\boldsymbol{r}}_0 + \epsilon \vec{\boldsymbol{v}}) - f(\vec{\boldsymbol{r}}_0)}{\epsilon}.$$

According to the above discussion, this derivative is just df/du along the tangent line, which according to the Master Formula is

$$D_{\vec{\boldsymbol{v}}} f = \vec{\boldsymbol{\nabla}} f \cdot \vec{\boldsymbol{v}}.$$

In Example 3 above, the left-hand side of (9.7.1) is just the directional derivative of h in the direction $\hat{\boldsymbol{T}}$, and could have been denoted by $D_{\hat{\boldsymbol{T}}} h$.

9.8 The Gradient in Curvilinear Coordinates

The master formula can be used to derive formulas for the gradient in other coordinate systems. We illustrate the method for polar coordinates.

In polar coordinates, we have

$$df = \frac{\partial f}{\partial s}\, ds + \frac{\partial f}{\partial \phi}\, d\phi$$

and of course

$$d\vec{\boldsymbol{r}} = ds\, \hat{\boldsymbol{s}} + r\, d\phi\, \hat{\boldsymbol{\phi}}$$

which is (8.3.1). Comparing these expressions with the Master Formula (9.1.2), we see immediately that we must have

$$\vec{\boldsymbol{\nabla}} f = \frac{\partial f}{\partial s}\, \hat{\boldsymbol{s}} + \frac{1}{s} \frac{\partial f}{\partial \phi}\, \hat{\boldsymbol{\phi}}. \tag{9.8.1}$$

Note the factor of $\frac{1}{s}$, which is needed to compensate for the factor of r in (8.3.1). Such factors are typical for the component expressions of vector derivatives in curvilinear coordinates.

Why would one want to compute the gradient in polar coordinates? Consider the computation of $\vec{\boldsymbol{\nabla}} \left(\ln \sqrt{x^2 + y^2} \right)$, which can done by brute force in rectangular coordinates; the calculation is straightforward but messy, even if you first use the properties of logarithms to remove the square root. Alternatively, using (9.8.1), it follows immediately that

$$\vec{\boldsymbol{\nabla}} \left(\ln \sqrt{x^2 + y^2} \right) = \vec{\boldsymbol{\nabla}} (\ln s) = \frac{1}{s}\, \hat{\boldsymbol{s}}.$$

A similar construction can be used to find the gradient in other coordinate systems. For instance, in cylindrical coordinates we have

$$dV = \frac{\partial V}{\partial s}\, ds + \frac{\partial V}{\partial y}\, d\phi + \frac{\partial V}{\partial z}\, dz$$

and since in cylindrical coordinates

$$d\vec{\boldsymbol{r}} = ds\, \hat{\boldsymbol{s}} + r\, d\phi\, \hat{\boldsymbol{\phi}} + dz\, \hat{\boldsymbol{z}}$$

[1] It is often assumed that $\vec{\boldsymbol{v}}$ is a unit vector, although this is not necessary.

we obtain

$$\vec{\boldsymbol{\nabla}} V = \frac{\partial V}{\partial s}\,\hat{\boldsymbol{s}} + \frac{1}{s}\frac{\partial V}{\partial \phi}\,\hat{\boldsymbol{\phi}} + \frac{\partial V}{\partial z}\,\hat{\boldsymbol{z}}$$

This formula, as well as similar formulas for other vector derivatives in rectangular, cylindrical, and spherical coordinates, are sufficiently important to the study of electromagnetism that they can, for instance, be found on the inside front cover of Griffiths' textbook, *Introduction to Electrodynamics*, and are also given in Appendix B.2.

Chapter 10

Integration

10.1 Review of Single Variable Integration

10.1.1 Theory

Integration is about chopping things up, and adding the pieces. This "chopping and adding" viewpoint is often helpful in setting up problems involving integration, and will be especially useful later for multiple integrals.

Figure 10.1.1 Chopping a line into small pieces.

For example, consider finding the total amount of chocolate on a straight piece of wafer (like a stick of Pocky), given the *density* of chocolate on the wafer. What does "density" mean? In this case, the amount of chocolate, which could be measured in grams, per unit distance along the wafer, which could be measured in centimeters. We call this quantity the *(linear) mass density* of chocolate on the wafer, which we will denote by λ. Using x to measure distance along the wafer, chop the wafer into small pieces of length dx, as indicated symbolically in Figure 10.1.1. [1] What is the mass of each piece? Clearly, $\lambda\,dx$. The total mass M of the chocolate on the wafer is given by adding up the mass of each piece. Since in general λ depends on position, it can be thought of as a function of x, that is, $\lambda = \lambda(x)$. Thus, "adding" really means "integrating", and we obtain

$$M = \int \lambda(x)\,dx. \tag{10.1.1}$$

You may have learned that integration is antidifferentiation, and that integrals are areas. Yes, the total amount of chocolate, thought of as a function of the distance from one end, is indeed an antiderivative of the function $\lambda(x)$. And yes, this integral represents the "area" under the graph of the function $\lambda(x)$, although the dimensions (mass) are not those of geometric area (length squared). But the "infinitesmal mass" $\lambda\,dx$ better represents the relevant physical process, and should therefore be regarded as fundamental. Note the importance of dx (and its units) to this argument!

From this point of view, the fundamental theorem of calculus is easy. If you add up little bits of choclate ($\lambda\,dx$), you get the total amount of chocolate.

[1] We prefer the use of differentials in this argument in order to emphasize that the pieces can be made as small as desired. This notation can be regarded as a shorthand for the use of Riemann sums involving Δx and an appropriate limit.

Similarly, if you add up the small changes in some quantity, say dq, the charge on a small piece of wire, you get its total change, so that

$$\int dq = q \tag{10.1.2}$$

which might look more familiar if you write $q = f(x)$, so that (10.1.2) becomes

$$\int \frac{df}{dx}\,dx = f. \tag{10.1.3}$$

Yes, this means that the integral of a derivative is the function you started with. In the chocolate example, that function is the "total chocolate" function, whose derivative is $\lambda(x)$. Nonetheless, what you're adding up is chocolate, that is, $\lambda\,dx$, not merely λ, which is the *density* of chocolate, not the *amount* of chocolate.

The use of differentials has other advantages. In the language of differentials, substitution is easy: If $u = x^2$, then $du = 2x\,dx$, so that e.g.

$$\int \cos(x^2)\,2x\,dx = \int \cos(u)\,du = \sin(u) = \sin(x^2). \tag{10.1.4}$$

And integration by parts is just the product rule: Start with

$$d(uv) = u\,dv + v\,du \tag{10.1.5}$$

and integrate both sides (and rearrange terms as needed).

All of the above integrals are *indefinite*; both sides of the equality are *functions*. *Definite* integrals are obtained simply by evaluating both sides at the endpoints of some interval. For example:

$$\int_a^b \frac{df}{dx}\,dx = f\Big|_a^b = f(b) - f(a) \tag{10.1.6}$$

and both sides of this equality are now *numbers* (with appropriate dimensions and units).

10.1.2 Practice

In practice, (10.1.2) tells us that (single) integration is nothing more than antidifferentation — just run the derivative rules backwards. Here are the basic derivative rules, in differential form:

$$\begin{aligned} d\left(u^n\right) &= nu^{n-1}\,du, \\ d\left(e^u\right) &= e^u\,du, \\ d(\sin u) &= \cos u\,du, \\ d(\cos u) &= -\sin u\,du, \\ d(\ln u) &= \frac{1}{u}\,du. \end{aligned}$$

To obtain the corresponding integration rules, simply integrate both sides, and use (10.1.2)). For example, the first rule becomes

$$\int nu^{n-1}\,du = u^n \tag{10.1.7}$$

which is more commonly written in the form

$$\int u^m \, du = \frac{u^{m+1}}{m+1} \tag{10.1.8}$$

where of course $m = n - 1 \neq -1$. [2]

10.1.3 Skills Check

At this point, you should be able to integrate easily simple expressions involving polynomials, trig, exponentials, and logarithms, including those requiring reasonably obvious substitutions, and you should be comfortable with occasional problems involving more complicated substitutions and/or integration by parts. If you are not comfortable with these skills, *including the necessary algebra*, you are strongly encouraged to spend as much time as needed on review and practice until you are truly fluent.

10.2 Scalar Line Integrals

What if you want to determine the mass of a wire in the shape of the curve C if you know the density λ? The same procedure still works; chop and add. In this case, the length of a small piece of the wire is $ds = |d\vec{\boldsymbol{r}}|$, so its mass is $\lambda \, ds$, and the integral becomes

$$m = \int_C \lambda \, ds \tag{10.2.1}$$

which can also be written as

$$m = \int_C \lambda(\vec{\boldsymbol{r}}) \, |d\vec{\boldsymbol{r}}| \tag{10.2.2}$$

which emphasizes both that λ is not constant, and that ds is the magnitude of $d\vec{\boldsymbol{r}}$.

Another standard application of this type of line integral is to find the *center of mass* of a wire. This is done by averaging the values of the coordinates, weighted by the density λ as follows:

$$\bar{x} = \frac{1}{m} \int_C x\lambda(\vec{\boldsymbol{r}}) \, ds \tag{10.2.3}$$

with m as defined above. Similar formulas hold for $\bar{y}$ and $\bar{z}$; the center of mass is then the point $(\bar{x}, \bar{y}, \bar{z})$.

10.3 Vector Line Integrals

Consider now the problem of finding the *work* W done by a force $\vec{\boldsymbol{F}}$ in moving a particle along a curve C. We begin with the relationship

$$\text{work} = \text{force} \times \text{distance}. \tag{10.3.1}$$

[2] It is customary, but by no means essential, to add an arbitrary constant to such integral formulas as a reminder that functions have many antiderivatives, which differ by a constant.

Suppose you take a small step $d\vec{\boldsymbol{r}}$ along the curve. How much work was done? Since only the component along the curve matters, we need to take the dot product of $\vec{\boldsymbol{F}}$ with $d\vec{\boldsymbol{r}}$. Adding this up along the curve yields

$$W = \int_C \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{r}}. \tag{10.3.2}$$

So how do you evaluate such an integral?
Use what you know!

10.4 General Surface Elements

Since surfaces are two-dimensional, chopping up a surface is usually done by drawing two families of curves on the surface. Then you can compute $d\vec{\boldsymbol{r}}$ on each family and take the cross product, see Section 1.21, to get the *vector surface element* in the form

$$d\vec{\boldsymbol{A}} = d\vec{\boldsymbol{r}}_1 \times d\vec{\boldsymbol{r}}_2. \tag{10.4.1}$$

In order to determine the area of the vector surface element, we need the magnitude of this expression, which is

$$dA = |d\vec{\boldsymbol{A}}| = |d\vec{\boldsymbol{r}}_1 \times d\vec{\boldsymbol{r}}_2| \tag{10.4.2}$$

and which is called the *(scalar) surface element*. This usage should remind you of the corresponding relation for line integrals, namely $ds = |d\vec{\boldsymbol{r}}|$.

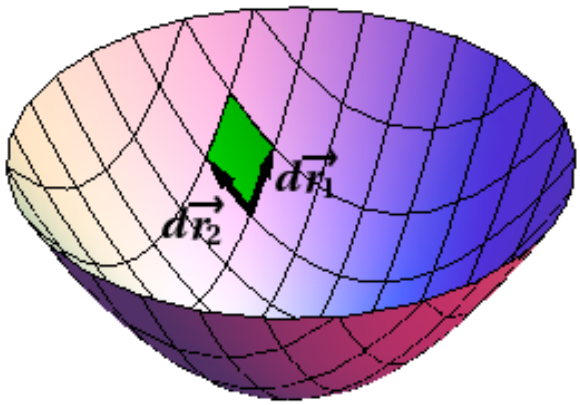


Figure 10.4.1 Chopping up a paraboloid in rectangular coordinates.

We illustrate this technique by computing the surface element for the paraboloid given by $z = x^2 + y^2$, as shown in Figure 10.4.1, with the two families of curves corresponding to $\{x = \text{const}\}$ and $\{y = \text{const}\}$. We start with the basic formula for the vector differential $d\vec{\boldsymbol{r}}$, namely

$$d\vec{\boldsymbol{r}} = dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}}. \tag{10.4.3}$$

What do you know? The expression for z leads to

$$dz = 2x\,dx + 2y\,dy. \tag{10.4.4}$$

In rectangular coordinates, it is natural to consider infinitesimal displacements in the x and y directions. In the x direction, y is constant, so $dy = 0$, and we obtain

$$d\vec{\boldsymbol{r}}_1 = dx\,\hat{\boldsymbol{x}} + 2x\,dx\,\hat{\boldsymbol{z}} = (\hat{\boldsymbol{x}} + 2x\,\hat{\boldsymbol{z}})\,dx. \tag{10.4.5}$$

Similarly, in the y direction, $dx = 0$, which leads to

$$d\vec{\boldsymbol{r}}_2 = dy\,\hat{\boldsymbol{y}} + 2y\,dy\,\hat{\boldsymbol{z}} = (\hat{\boldsymbol{y}} + 2y\,\hat{\boldsymbol{z}})\,dy. \tag{10.4.6}$$

Putting this together, we obtain

$$\begin{aligned} d\vec{\boldsymbol{A}} = d\vec{\boldsymbol{r}}_1 \times d\vec{\boldsymbol{r}}_2 &= (\hat{\boldsymbol{x}} + 2x\,\hat{\boldsymbol{z}}) \times (\hat{\boldsymbol{y}} + 2y\,\hat{\boldsymbol{z}})\,dx\,dy \\ &= (-2x\,\hat{\boldsymbol{x}} - 2y\,\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})\,dx\,dy \end{aligned} \tag{10.4.7}$$

for the vector surface element, and

$$dA = |-2x\,\hat{\boldsymbol{x}} - 2y\,\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}|\,dx\,dy = \sqrt{1 + 4x^2 + 4y^2}\,dx\,dy \tag{10.4.8}$$

for the scalar surface element. Can you repeat this computation in cylindrical coordinates? (See Section 11.4 for the answer.)

This construction emphasizes that "area" is really a *vector*, whose direction is perpendicular to the surface, and whose magnitude is the area. Note that there are always *two* choices for the direction; choosing one determines the *orientation* of the surface.

When using (10.4.1) and (10.4.2), it doesn't matter how you chop up the surface. It is of course possible to get the opposite orientation, for instance by interchanging the roles of $d\vec{\boldsymbol{r}}_1$ and $d\vec{\boldsymbol{r}}_2$. Rather than worrying too much about getting the "right" orientation from the beginning, it is usually simpler to check after you've calculated $d\vec{\boldsymbol{S}}$ whether the orientations you've got agrees with the requirements of the problem. If not, insert a minus sign.

Just as a curve is a 1-dimensional set of points, a surface is 2-dimensional. When computing line integrals, it was necessary to write everything in terms of a single parameter before integrating. Similarly, for surface integrals you must write everything, including the limits of integration, in terms of exactly *two* parameters before starting to integrate.

Finally, a word about notation. You will often see dS instead of dA, and $d\vec{\boldsymbol{S}}$ instead of $d\vec{\boldsymbol{A}}$; most authors use dA in the xy-plane.

10.5 Vector Surface Elements

In this section, you will find the vector surface elements for common shapes with high symmetry.

Activity 10.5.1 Surface Elements for Planes, Cylinders, and Spheres. Using the general formula for the scalar surface elements from Section (10.5.1) or the vector surface element

$$d\vec{\boldsymbol{A}} = d\vec{\boldsymbol{r}}_1 \times d\vec{\boldsymbol{r}}_2 \tag{10.5.1}$$

find explicit formulas for the vector surface element in each of the following cases:

- a plane in both rectangular and polar coordinates;
- the three surfaces (top, bottom, and curved side) of a cylinder with finite length;
- the surface of a sphere.

Answer. In this activity, you should have obtained the following common surface elements:

$$\text{(plane)} \quad z = \text{ const}: \qquad d\vec{\boldsymbol{A}} = dx\,dy\,\hat{\boldsymbol{z}};$$

$$\begin{aligned}
&\text{(plane)} && z = \text{ const}: && d\vec{\boldsymbol{A}} = s\,ds\,d\phi\,\hat{\boldsymbol{z}};\\
&\text{(top of cylinder)} && z = \text{ const}: && d\vec{\boldsymbol{A}} = s\,ds\,d\phi\,\hat{\boldsymbol{z}};\\
&\text{(bottom of cylinder)} && z = \text{ const}: && d\vec{\boldsymbol{A}} = -s\,ds\,d\phi\,\hat{\boldsymbol{z}};\\
&\text{(side of cylinder)} && s = \text{ const}: && d\vec{\boldsymbol{A}} = s\,d\phi\,dz\,\hat{\boldsymbol{s}};\\
&\text{(sphere)} && r = \text{ const}: && d\vec{\boldsymbol{A}} = r^2\sin\theta\,d\theta\,d\phi\,\hat{\boldsymbol{r}}.
\end{aligned}$$

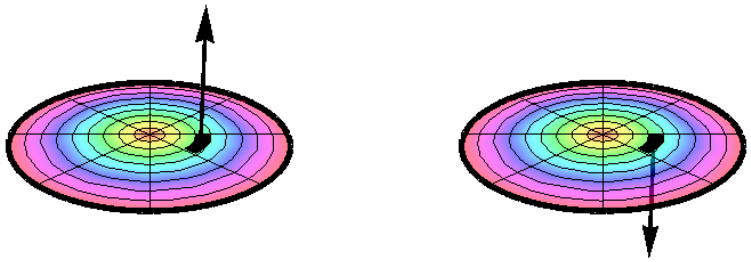


Figure 10.5.1 A disk oriented upward (left) and downward (right).

In each of these examples, the direction of the vector surface element is given by the basis vector associated with the coordinate that you held constant when describing the surface — up to sign. This sign corresponds to a choice about the orientation of the surface. The standard conventions, adopted above, are to orient the surface element *outward* for a closed surface such as a sphere, and *upward* otherwise, unless otherwise stated. In the absence of such a convention, each of the surface elements above would have to be preceded by a factor of ± 1. Compare the two drawings in Figure 10.5.1.

When using formula (10.5.1), the choice of orientation is determined by the order in which $d\vec{\boldsymbol{r}}_1$ and $d\vec{\boldsymbol{r}}_2$ are multiplied. By convention, one usually computes $d\vec{\boldsymbol{A}} = d\vec{\boldsymbol{r}}_1 \times d\vec{\boldsymbol{r}}_2$, so the orientation is determined by the choice of which vector is $d\vec{\boldsymbol{r}}_1$, and which is $d\vec{\boldsymbol{r}}_2$. It is up to you to *choose* this labeling to correctly match the desired orientation. Which orientation is determined by the choices shown in Figures 10.4.1 and Figure 11.4.1?

Formula (10.5.1) will work for all kinds of complicated surfaces, so we wanted you to get practice in learning how to use it. However, when a surface can be described as a "coordinate equals constant" surface in an orthogonal coordinate system, then the cross product is trivial. You can think of the *scalar* area element as an infinitesimal "rectangle" whose area is just the product of the infinitesimal lengths of the two sides.

10.6 Scalar Surface Integrals

Consider again the example in Section 11.1, which involved the part of the plane $x + y + z = 1$ which lies in the first quadrant. Suppose you want to find the average height of this triangular region above the xy-plane. To do this, chop the surface into small pieces, each at height $z = 1 - x - y$. In order to compute the average height, we need to find

$$\text{avg height} = \frac{1}{\text{area}} \int_S z\,dA \tag{10.6.1}$$

where the total area of the surface can be found either as

$$\text{area} = \int_S dA \tag{10.6.2}$$

or from simple geometry. So we need to determine dA. But we already know $d\vec{\boldsymbol{A}}$ for this surface from (11.1.5)! It is therefore straightforward to compute

$$dA = |d\vec{\boldsymbol{A}}| = |\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}|\, dx\, dy = \sqrt{3}\, dx\, dy \tag{10.6.3}$$

and therefore

$$\text{avg height} = \frac{1}{\sqrt{3}/2} \int_0^1 \int_0^{1-x} (1 - x - y)\sqrt{3}\, dy\, dx = \frac{1}{3}. \tag{10.6.4}$$

10.7 Volume Integrals

The basic building block for volume integrals is the infinitesimal volume, obtained by chopping up the volume into small "parallelepipeds". Our approach for surface integrals can be extended to volume integrals using the triple product. The volume element becomes

$$d\tau = (d\vec{\boldsymbol{r}}_1 \times d\vec{\boldsymbol{r}}_2) \cdot d\vec{\boldsymbol{r}}_3 \tag{10.7.1}$$

for the $d\vec{\boldsymbol{r}}$'s computed for (any!) 3 non-coplanar families of curves. [1] (The volume element is often written as dV, but we prefer $d\tau$ to avoid confusion with the electrostatic potential V.) Using the natural families of curves in spherical coordinates, we could take

$$d\vec{\boldsymbol{r}}_1 = r\, d\theta\, \hat{\boldsymbol{\theta}}$$
$$d\vec{\boldsymbol{r}}_2 = r\, \sin\theta\, d\phi\, \hat{\boldsymbol{\phi}}$$

as before, and add

$$d\vec{\boldsymbol{r}}_3 = dr\, \hat{\boldsymbol{r}} \tag{10.7.2}$$

leading to

$$d\tau = r^2 \sin\theta\, dr\, d\theta\, d\phi \tag{10.7.3}$$

as expected. For any orthogonal coordinate system, this method is of course equivalent to visualizing a small coordinate box, and multiplying the lengths of the three sides.

[1] The triple product has a cyclic symmetry, but the orientation matters — the order must be chosen so that $d\tau$ is positive.

Chapter 11

Vector Surface Integrals

11.1 Flux

At any give point along a curve, there is a natural vector, namely the (unit) tangent vector $\hat{\boldsymbol{T}}$. Therefore, it is natural to add up the *tangential* component of a given vector field along a curve. When the vector field represents force, this integral represents the work done by the force along the curve. But there is no natural tangential direction at a point on a surface, or rather there are too many of them. The natural vector at a point on a surface is the (unit) *normal* vector $\hat{\boldsymbol{n}}$, so on a surface it is natural to add up the normal component of a given vector field; this integral is known as the *flux* of the vector field through the surface.

We already know that the vector surface element is given by

$$d\vec{\boldsymbol{A}} = d\vec{\boldsymbol{r}}_1 \times d\vec{\boldsymbol{r}}_2. \tag{11.1.1}$$

Since $d\vec{\boldsymbol{r}}_1$ and $d\vec{\boldsymbol{r}}_2$ are both tangent to the surface, $d\vec{\boldsymbol{A}}$ is perpendicular to the surface, and is therefore often written

$$d\vec{\boldsymbol{A}} = \hat{\boldsymbol{n}}\, dA. \tag{11.1.2}$$

Putting this all together, the flux of a vector field $\vec{\boldsymbol{F}}$ through the surface is given by

$$\text{flux of } \vec{\boldsymbol{F}} \text{ through } S = \int_S \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{A}}. \tag{11.1.3}$$

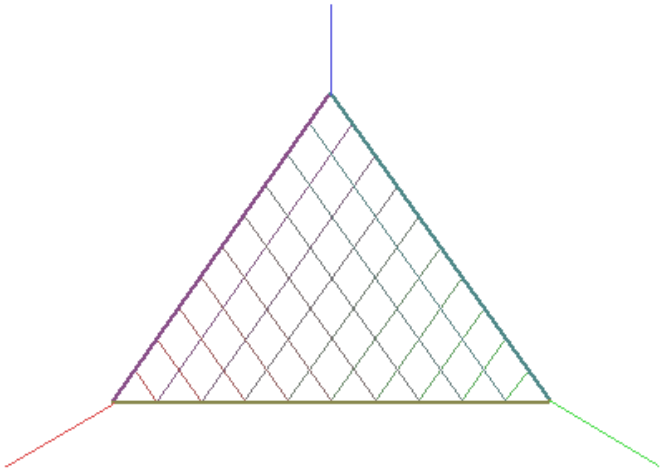


Figure 11.1.1 A triangular region in the first octant, chopped parallel to the x- and y-axes.

We first consider a problem typical of those in calculus textbooks, namely finding the flux of the vector field $\vec{\boldsymbol{F}} = z\,\hat{\boldsymbol{z}}$ up through the part of the plane $x+y+z=1$ lying in the first octant, as shown in Figure 11.1.1. We begin with the infinitesimal vector displacement in rectangular coordinates in 3 dimensions, namely

$$d\vec{\boldsymbol{r}} = dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}}. \tag{11.1.4}$$

A natural choice of curves in this surface is given by setting y or x constant, so that $dy = 0$ or $dx = 0$, respectively. On the surface, we have $dx + dy + dz = 0$, which we can use to eliminate one variable along each of these curves. We thus obtain

$$\begin{aligned} d\vec{\boldsymbol{r}}_1 &= dx\,\hat{\boldsymbol{x}} + dz\,\hat{\boldsymbol{z}} = (\hat{\boldsymbol{x}} - \hat{\boldsymbol{z}})\,dx, \\ d\vec{\boldsymbol{r}}_2 &= dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}} = (\hat{\boldsymbol{y}} - \hat{\boldsymbol{z}})\,dy, \end{aligned}$$

where we have used what we know (the equation of the plane) to determine each expression in terms of a single parameter. The surface element is thus

$$d\vec{\boldsymbol{A}} = d\vec{\boldsymbol{r}}_1 \times d\vec{\boldsymbol{r}}_2 = (\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})\,dx\,dy \tag{11.1.5}$$

and the flux becomes [1]

$$\begin{aligned} \int_S \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{A}} &= \int_S z\,dx\,dy \\ &= \int_0^1 \int_0^{1-y} (1-x-y)\,dx\,dy = \frac{1}{6}. \end{aligned} \tag{11.1.6}$$

The limits were chosen by visualizing the projection of the surface into the xy-plane, which is a triangle bounded by the x-axis, the y-axis, and the line whose equation is $x+y=1$. Note that this latter equation is obtained from the equation of the surface by using what we know, namely that $z=0$.

Just as for line integrals, there is a rule of thumb which tells you when to stop using what you know to compute surface integrals: Don't start integrating until the integral is expressed in terms of *two* parameters, and the limits in terms of those parameters have been determined. Surfaces are two-dimensional!

[1] Some readers will prefer to change the domain of integration in the second integral to be the projection of S into the xy-plane. We prefer to integrate over the actual surface whenever possible.

11.2 Dot Products and Components

A field can be expressed in many different coordinate systems. For example, in rectangular coordinates, the electric field is

$$\vec{\boldsymbol{E}} = E_x\,\hat{\boldsymbol{x}} + E_y\,\hat{\boldsymbol{y}} + E_z\,\hat{\boldsymbol{z}}.$$

Similarly, in cylindrical coordinates,

$$\vec{\boldsymbol{E}} = E_s\,\hat{\boldsymbol{s}} + E_\phi\,\hat{\boldsymbol{\phi}} + E_z\,\hat{\boldsymbol{z}}.$$

What is the x-component of $\vec{\boldsymbol{E}}$? Surely just E_x. The s-component? E_s.

How could you find these components, given $\vec{\boldsymbol{E}}$? The (scalar) component of a vector field in a given direction is just the projection in that direction. Projections are dot products. Thus,

$$E_x = \vec{\boldsymbol{E}} \cdot \hat{\boldsymbol{x}}$$

and

$$E_s = \vec{\boldsymbol{E}} \cdot \hat{\boldsymbol{s}}.$$

Given a surface, it makes sense to ask what the component $E_\perp$ of the electric field is, perpendicular to the surface. By the same reasoning, we have

$$E_\perp = \vec{\boldsymbol{E}} \cdot \hat{\boldsymbol{n}}$$

where $\hat{\boldsymbol{n}}$ is the unit normal to the surface.

The component parallel to the surface, $E_\parallel$ is more subtle, since there are an infinite number of directions parallel to the surface. One way around this problem is to speaks of *vector components*, by attaching the direction to the scalar component. For instance

$$\vec{\boldsymbol{E}}_\perp = E_\perp\,\hat{\boldsymbol{n}}.$$

We can now define the parallel (vector) component of $\vec{\boldsymbol{E}}$ as the vector that is left after the perpendicular component is subtracted

$$\vec{\boldsymbol{E}}_\parallel = \vec{\boldsymbol{E}} - \vec{\boldsymbol{E}}_\perp$$

from which the magnitude $E_\parallel = |\vec{\boldsymbol{E}}_\parallel|$ can be computed using the Pythagorean Theorem if desired.

11.3 Highly Symmetric Surfaces

One of the most fundamental examples in electromagnetism is the electric field of a point charge.

The electric field of a point charge q at the origin is given by

$$\vec{\boldsymbol{E}} = \frac{q}{4\pi\epsilon_0}\frac{\hat{\boldsymbol{r}}}{r^2} = \frac{q}{4\pi\epsilon_0}\frac{x\,\hat{\boldsymbol{x}} + y\,\hat{\boldsymbol{y}} + z\,\hat{\boldsymbol{z}}}{(x^2+y^2+z^2)^{3/2}} \tag{11.3.1}$$

where $\hat{\boldsymbol{r}}$ is now the unit vector in the radial direction in *spherical* coordinates. The first expression clearly indicates both the spherical symmetry of $\vec{\boldsymbol{E}}$ and its $\frac{1}{r^2}$ fall-off behavior, whereas the second expression does neither. Given the

electric field, Gauss' Law allows one to determine the total charge inside any closed surface, namely

$$\frac{q}{\epsilon_0} = \int_S \vec{\boldsymbol{E}} \cdot d\vec{\boldsymbol{A}} \tag{11.3.2}$$

which is of course just the Divergence Theorem.

It is easy to determine $d\vec{\boldsymbol{A}}$ on the sphere by inspection; we nevertheless go through the details of the differential approach for this case. We use "physicists' conventions" for spherical coordinates, so that θ is the angle from the North Pole, and ϕ the angle in the xy-plane. We use the obvious families of curves, namely the lines of latitude and longitude. Starting either from the general formula for $d\vec{\boldsymbol{r}}$ in spherical coordinates, namely

$$d\vec{\boldsymbol{r}} = dr\,\hat{\boldsymbol{r}} + r\,d\theta\,\hat{\boldsymbol{\theta}} + r\sin\theta\,d\phi\,\hat{\boldsymbol{\phi}}, \tag{11.3.3}$$

or directly using the geometry behind that formula, one quickly arrives at

$$\begin{aligned} d\vec{\boldsymbol{r}}_1 &= r\,d\theta\,\hat{\boldsymbol{\theta}}, \\ d\vec{\boldsymbol{r}}_2 &= r\sin\theta\,d\phi\,\hat{\boldsymbol{\phi}}, \\ d\vec{\boldsymbol{A}} &= d\vec{\boldsymbol{r}}_1 \times d\vec{\boldsymbol{r}}_2 = r^2\sin\theta\,d\theta\,d\phi\,\hat{\boldsymbol{r}}, \end{aligned}$$

so that

$$\int_S \vec{\boldsymbol{E}} \cdot d\vec{\boldsymbol{A}} = \int_0^{2\pi}\int_0^{\pi} \frac{q}{4\pi\epsilon_0}\frac{\hat{\boldsymbol{r}}}{r^2} \cdot r^2\sin\theta\,d\theta\,d\phi\,\hat{\boldsymbol{r}} = \frac{q}{\epsilon_0} \tag{11.3.4}$$

as expected.

11.4 Less Symmetric Surfaces

The reader may have the feeling that two quite different languages are being spoken here. The tilted plane in Section 11.1 was treated in essentially the traditional manner found in calculus textbooks, using rectangular coordinates. While the "use what you know" strategy may be somewhat unfamiliar, the basic idea should not be. On the other hand, the examples in Section 11.3 will be quite unfamiliar to most mathematicians, due to their use of adapted basis vectors such as $\hat{\boldsymbol{r}}$. Mastering these examples helps develop experience looking for symmetry and making geometric arguments. At the same time, not all problems have symmetry!

We argue, however, that the approach being presented here is much more flexible than may appear at first sight. We demonstrate this flexibility by integrating over a paraboloid, the classic example found in calculus textbooks.

We compute the flux of the axially symmetric vector field

$$\vec{\boldsymbol{F}} = s\,\hat{\boldsymbol{s}} = x\,\hat{\boldsymbol{x}} + y\,\hat{\boldsymbol{y}} \tag{11.4.1}$$

"outwards" through the part of the paraboloid $z = s^2$ lying below the plane $z = 4$. The first thing we need is the formula for $d\vec{\boldsymbol{r}}$ in cylindrical coordinates, which is a straightforward generalization of (8.3.1) in polar coordinates, namely

$$d\vec{\boldsymbol{r}} = ds\,\hat{\boldsymbol{s}} + s\,d\phi\,\hat{\boldsymbol{\phi}} + dz\,\hat{\boldsymbol{z}}. \tag{11.4.2}$$

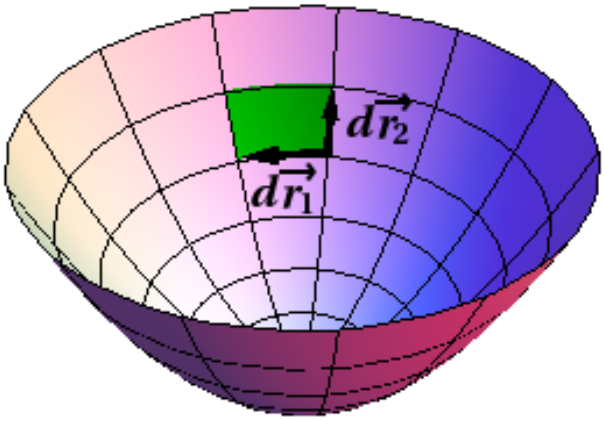


Figure 11.4.1 Chopping up a paraboloid in rectangular coordinates.

Next, we need two families of curves on the paraboloid; the natural choices are those with r = constant or ϕ = constant, respectively, as shown in Figure 11.4.1. If s is constant, so is z, and we have simply

$$d\vec{\boldsymbol{r}}_1 = s\,d\phi\,\hat{\boldsymbol{\phi}}. \tag{11.4.3}$$

If ϕ is constant, there will be no $\hat{\boldsymbol{\phi}}$ term in $d\vec{\boldsymbol{r}}_2$, but we must still use what we know to compute $dz = 2s\,ds$, thus obtaining

$$d\vec{\boldsymbol{r}}_2 = ds\,\hat{\boldsymbol{s}} + 2s\,ds\,\hat{\boldsymbol{z}}. \tag{11.4.4}$$

Taking the cross product leads to (compare (10.4.7))

$$d\vec{\boldsymbol{A}} = d\vec{\boldsymbol{r}}_1 \times d\vec{\boldsymbol{r}}_2 = (2s^2\,\hat{\boldsymbol{s}} - s\hat{\boldsymbol{z}})\,ds\,d\phi \tag{11.4.5}$$

and at this point we must check that we have chosen the correct orientation. (We have, since the coefficient of $\hat{\boldsymbol{z}}$ is *negative*.) The rest is easy: Compute the dot product, determine the limits, and do the integral. This results in

$$\int_S \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{A}} = \int_0^{2\pi} \int_0^2 2s^3\,ds\,d\phi = 16\pi. \tag{11.4.6}$$

It is of course also possible to use rectangular coordinates to determine $d\vec{\boldsymbol{A}}$, choosing curves on the paraboloid $z = x^2 + y^2$ with x = constant or y = constant. The resulting integral cries out for polar coordinates — which turns it into the same integral as the above.

There is however a significant difference between these two approaches: Drawing the curves on the paraboloid with s or ϕ held constant is easy; drawing the curves with x or y held constant is not. Try it! [1] The rectangular coordinate approach relies for its geometric intuition on the generic figure found in most textbooks which maps the rectangular "parameter space" into the surface, whereas the cylindrical coordinate approach starts by choosing the geometrically obvious curves in the given surface.

[1] Most graphing packages, such as Maple, will automatically draw the latter set of curves for you. It is not always straightforward to get them to draw the former instead!

Chapter 12

Derivatives of Vector Fields

12.1 The Definition of Divergence

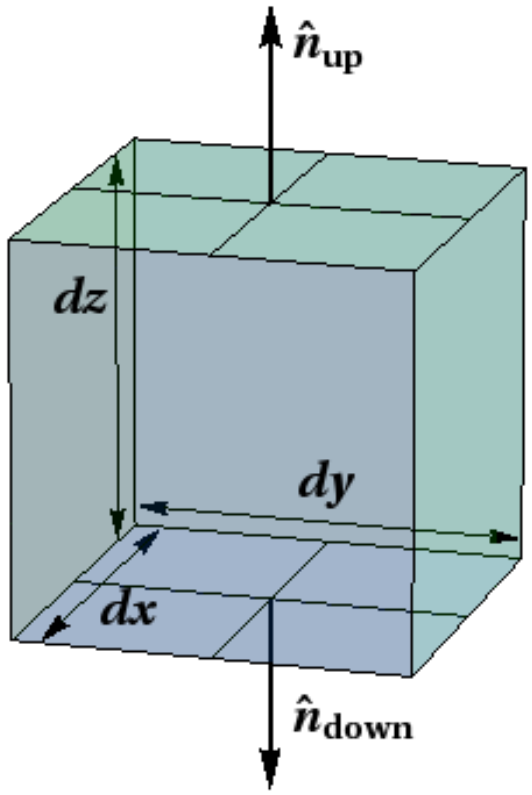


Figure 12.1.1 Computing the vertical contribution of the flux through a small rectangular box.

Consider a small closed box, with sides parallel to the coordinate planes, as shown in Figure 12.1.1. What is the flux of an arbitrary vector field $\vec{F}$ out of

the box?

Consider first the vertical contribution, namely the flux *up* through the top plus the flux *down* through the bottom. These two sides each have area element $dA = dx\,dy$, but the outward normal vectors point in opposite directions, that is

$$\begin{aligned}\hat{\boldsymbol{n}}_{\text{up}} &= \hat{\boldsymbol{z}},\\ \hat{\boldsymbol{n}}_{\text{down}} &= -\hat{\boldsymbol{z}},\end{aligned}$$

so we get

$$\begin{aligned}\sum_{\text{top+bottom}} \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{A}} &= \vec{\boldsymbol{F}}(z+dz)\cdot\hat{\boldsymbol{z}}\,dx\,dy - \vec{\boldsymbol{F}}(z)\cdot\hat{\boldsymbol{z}}\,dx\,dy\\ &= \Big(F_z(z+dz) - F_z(z)\Big)\,dx\,dy\\ &= \frac{F_z(z+dz)-F_z(z)}{dz}\,dx\,dy\,dz\\ &= \frac{\partial F_z}{\partial z}\,dx\,dy\,dz\end{aligned}$$

where we have multiplied and divided by dz to obtain the volume element $d\tau = dx\,dy\,dz$ in the third step, and used the limit definition of the derivative in the final step.

Repeating this argument using the remaining pairs of faces, it follows that the total flux out of the box is

$$\text{total flux} = \sum_{\text{box}} \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{A}} = \left(\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}\right)\,d\tau.$$

Since the total flux is proportional to the volume of the box, it approaches zero as the box shrinks down to a point. The interesting quantity is therefore the ratio of the flux to volume; this ratio is called the divergence.

At any point P, we therefore define the *divergence* of a vector field $\vec{\boldsymbol{F}}$, written $\vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{F}}$, to be the flux of $\vec{\boldsymbol{F}}$ per unit volume leaving a small box around P. In other words, the divergence is the limit as the box collapses around P of the ratio of the flux of the vector field out of the box to the volume of the box. Thus, the divergence of $\vec{\boldsymbol{F}}$ at P is the flux per unit volume through a small box around P, which is given in rectangular coordinates by

$$\vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{F}} = \frac{\text{flux}}{\text{unit volume}} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}.$$

You may have seen this formula before, but remember that it is merely the rectangular coordinate expression for the divergence of $\vec{\boldsymbol{F}}$; the divergence is defined geometrically as flux per unit volume. Similar computations can be used to determine expressions for the divergence in other coordinate systems, see Section B.2 for a sketch of the derivation and Appendix B.2 for the formulas. Because of the geometric nature of divergence, these expressions turn out to give the same value at each point in space.

12.2 The Divergence in Two Dimensions

Although the divergence is usually discussed in three dimensions, the construction in Section 12.1 can also be used in two dimensions. The only significant change is that a new type of *flux* must be defined on curves, rather than surfaces.

If C is a (simple) closed curve in the plane, it has an inside and an outside. If the *outward* normal vector is $\hat{\boldsymbol{n}}$, then the *flux* of a vector field $\vec{\boldsymbol{E}}$ out of C is given by

$$\text{flux} = \int_C \vec{\boldsymbol{E}} \cdot \hat{\boldsymbol{n}}\, ds$$

where $ds = |d\vec{\boldsymbol{r}}|$ denotes infinitesimal arclength.

Applying the argument in Section 12.1 to a small rectangular box yields essentially the same result, namely that the total flux out of the (two-dimensional) box is some sort of derivative, times the *area* of the box. Thus, in two dimensions we define

$$\vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{E}} = \frac{\text{flux}}{\text{unit area}}$$

and obtain the rectangular coordinate expression

$$\vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{E}} = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y}.$$

When discussing the properties of the divergence, two-dimensional examples are often given, in part because they are easier to interpret (and to draw!). Such examples can always be interpreted using the two-dimensional notions of flux and divergence given in this section, so long as care is taken to note the different units (area vs. volume) in the two- and three-dimensional cases. Alternatively, two-dimensional examples can be interpreted as a horizontal slice of a three-dimensional example, in which the vector field is also horizontal (no $\hat{\boldsymbol{z}}$ component), so that there is no flux through the top and bottom faces of the box. In this interpretation, the height of the box does not affect the computation, but nonetheless restores the units of flux per unit volume to the divergence.

The vector fields in Figure 12.2.1 model this behavior. They appear to be two-dimensional, but are really three-dimensional, as can be seen by clicking on them and rotating the images. (You may wish to zoom out first, using the scroll wheel of your mouse, or by right-clicking and selecting "Zoom to fit".)

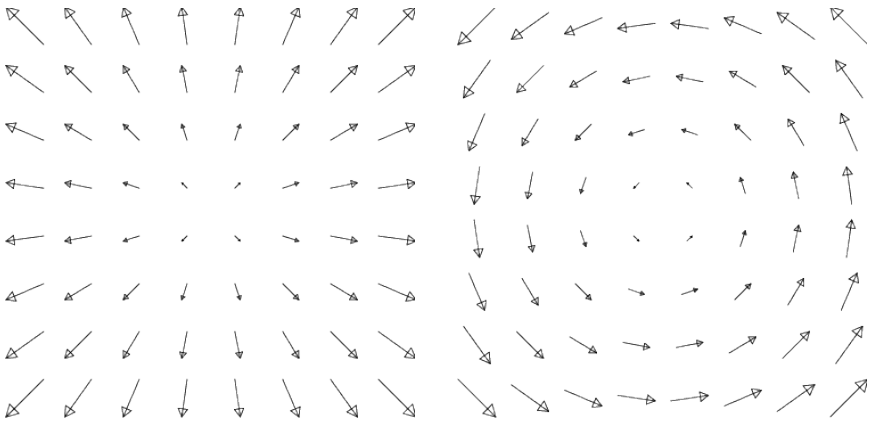


Figure 12.2.1 Interpreting (horizontal) vector fields as two dimensional.

12.3 Exploring the Divergence

Figure 12.3.1 below shows the relationship between flux and divergence in two dimensions. You can choose the vector field $\vec{\boldsymbol{v}}$ by entering its components v_x and v_y, move the box by dragging its center, and change the size s of the box by moving the slider.

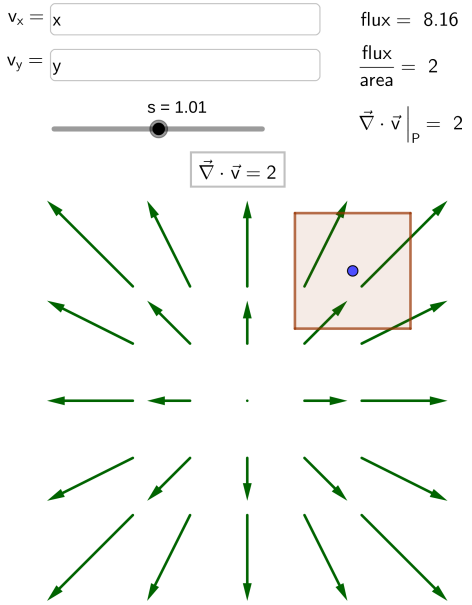


Figure 12.3.1 The relationship between flux and divergence.

Activity 12.3.1 Exploring Divergence. Enter the (two-dimensional vector field of your choice into the applet in Figure 12.3.1 by entering its components. Determine the flux per unit area at several locations by moving the box and adjusting the slider. In each case, compare your result (shown in the applet as $\frac{\text{flux}}{\text{area}}$) with the computed value of the divergence at the center of the box (shown as $\vec{\nabla} \cdot \vec{v}\big|_P$).

What do you notice?

Hint. Start with vector fields whose components are linear functions of x and y, then try more complicated functions.

12.4 The Divergence in Curvilinear Coordinates

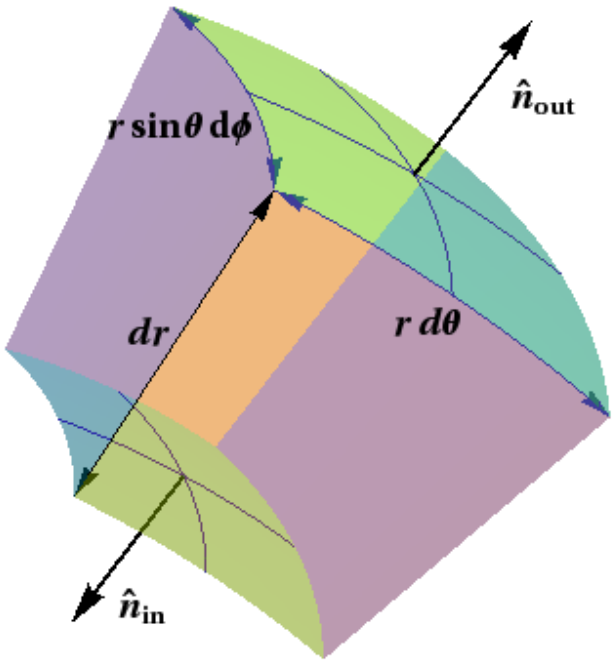


Figure 12.4.1 Computing the radial contribution to the flux through a small box in spherical coordinates.

The divergence is defined in terms of flux per unit volume. In Section 12.1, we used this geometric definition to derive an expression for $\vec{\nabla}\cdot\vec{F}$ in rectangular coordinates, namely

$$\vec{\nabla}\cdot\vec{F} = \frac{\text{flux}}{\text{unit volume}} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}.$$

Similar computations to those in rectangular coordinates can be done using boxes adapted to other coordinate systems. Not surprisingly, this introduces some additional scale factors such as r and $\sin\theta$. For instance, consider a radial vector field of the form

$$\vec{E} = E_r\,\hat{r}$$

where $\hat{r}$ is the unit vector in the radial direction. The electric field of a point charge would have this form. What is the flux of $\vec{E}$ through a small box around an arbitrary point P, whose sides are surfaces with one of the spherical coordinates held constant, as shown in Figure 12.4.1? Only the two sides which are parts of spheres contribute, and each such contribution takes the form

$$\vec{E}\cdot d\vec{A} = \pm E_r\, r^2 \sin\theta\, d\theta\, d\phi.$$

An argument similar to the one used in rectangular coordinates leads to

$$\vec{E}\cdot d\vec{A} = \frac{\partial}{\partial r}\left(r^2 E_r\right)\sin\theta\, dr\, d\theta\, d\phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 E_r\right) d\tau$$

where it is important to note that the factor of r^2 must also be differentiated. It now finally follows that

$$\vec{\nabla} \cdot \vec{E} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 E_r \right).$$

This expression only gives the divergence of the very special vector field $\vec{E}$ given above. The full expression for the divergence in spherical coordinates is obtained by performing a similar analysis of the flux of an arbitrary vector field $\vec{F}$ through our small box; the result can be found in Appendix B.2. This formula, as well as similar formulas for other vector derivatives in rectangular, cylindrical, and spherical coordinates, are sufficiently important to the study of electromagnetism that they can, for instance, be found on the inside front cover of Griffiths' textbook, *Introduction to Electrodynamics*.

12.5 Exploring the Divergence in Polar Coordinates

Figure 12.5.1 below shows the relationship between flux and divergence using polar coordinates and basis vectors. You can choose the vector field $\vec{v}$ by entering its components v_r and v_ϕ, move the box by dragging its center, and change the size s of the box by moving the slider.

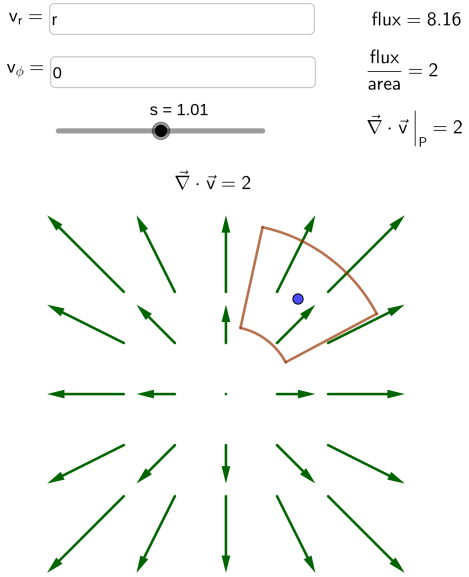


Figure 12.5.1 The relationship between flux and divergence.

Activity 12.5.1 Exploring Divergence. Enter the (two-dimensional vector field of your choice into the applet in Figure 12.5.1 by entering its components. Determine the flux per unit area at several locations by moving the box and adjusting the slider. In each case, compare your result (shown in the applet as $\frac{\text{flux}}{\text{area}}$) with the computed value of the divergence at the center of the box (shown as $\vec{\nabla} \cdot \vec{v}\big|_P$).

What do you notice?

Hint. Start with vector fields whose components are linear functions of r, then try more complicated functions.

12.6 Visualizing Divergence

Recall that

$$\vec{\nabla} \cdot \vec{F} \approx \frac{\int \vec{F} \cdot d\vec{A}}{\text{volume of box}} = \frac{\text{flux}}{\text{unit volume}} \tag{12.6.1}$$

so that the divergence measures how much a vector field "points out" of a box.

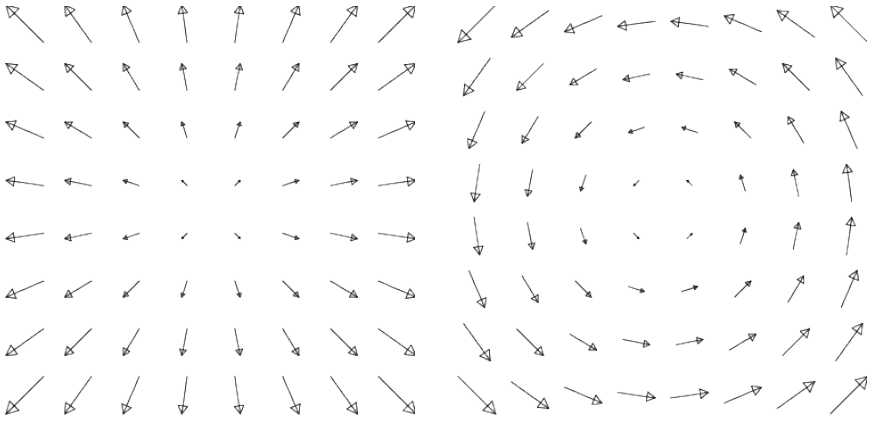


Figure 12.6.1 Two vector fields.

Can we use these ideas to investigate graphically the divergence of a given vector field?

Activity 12.6.1 The Geometry of Divergence. Consider the two vector fields in Figure 12.6.1. In each case, can you find the divergence?

Hint. A natural place to start is at the origin. So draw a small box around the origin, as shown in Figure 12.6.2. [1] Is there flux across the loop?

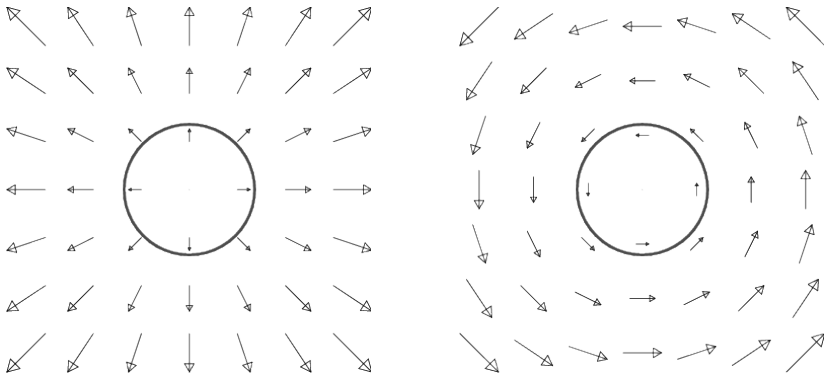


Figure 12.6.2 The same two vector fields, with loops at the origin.

The figures above help us determine the divergence *at the origin*, but not elsewhere. The divergence is a function, which can vary from point to point. We therefore need to examine loops which are *not* at the origin. It is useful to adapt the shape of our loop to the vector field under consideration. Both of our vector fields are better adapted to polar coordinates than to rectangular coordinates, so we use polar boxes. Can you determine the divergence using the loops in Figure 12.6.3? Imagine trying to do the same thing with a rectangular loop, or even a circular loop.

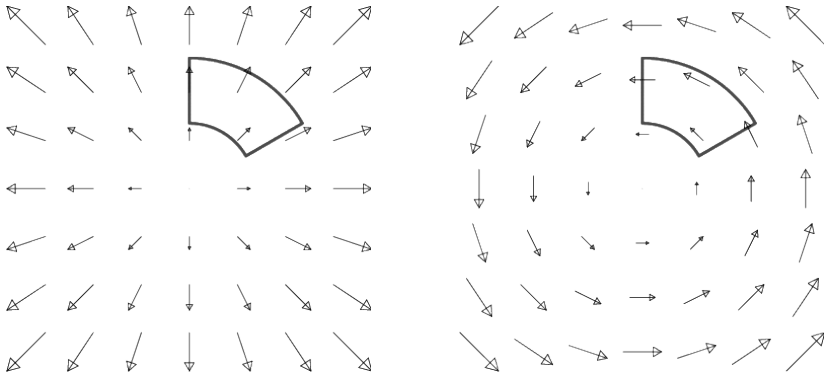


Figure 12.6.3 The same two vector fields, with loops not at the origin.

Finally, it is important to realize that not all vector fields which point away from the origin have divergence. The example in Figure 12.6.4 demonstrates this important principle; it has no divergence away from the origin. This figure represents a solution of Maxwell's equations for electromagnetism, and describes the electric field of an infinite charged wire

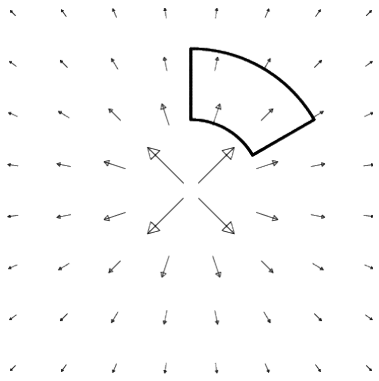


Figure 12.6.4 One more vector field.

12.7 The Divergence Theorem

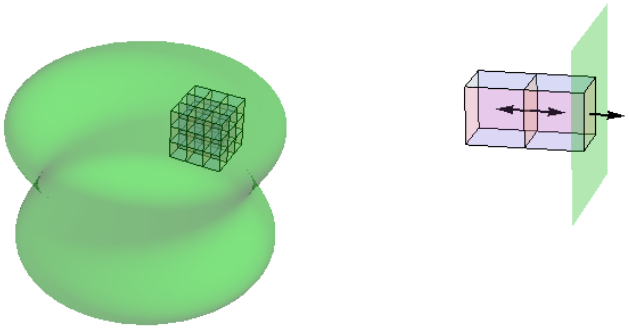


Figure 12.7.1 The geometry of the Divergence Theorem.

[1] In two dimensions, both "boxes" are loops. In three dimensions, the oriented box used to measure circulation is still a loop, but the box used to measure flux is now an ordinary, 3-dimensional box.

The total flux of a vector field $\vec{\boldsymbol{F}}$ out through a small rectangular box is

$$\text{flux} = \sum_{\text{box}} \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{A}} = \vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{F}}\, d\tau$$

But any closed region can be filled with such boxes, as shown in the first diagram in Figure 12.7.1. Furthermore, the flux out of such a region is just the sum of the fluxes out of each of the smaller boxes, since the net flux through any common face will be zero (because adjacent boxes have opposite notions of "out of"), as indicated schematically in the second diagram in Figure 12.7.1. Thus, the total flux out of any closed box is given by

$$\int_{\text{box}} \vec{\boldsymbol{F}} \cdot d\vec{\boldsymbol{A}} = \int_{\text{inside}} \vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{F}}\ d\tau.$$

This relation is known as the *Divergence Theorem*.

12.8 The Geometry of Curl

Put a paddlewheel into a moving body of water. Depending on the details of the flow, the paddlewheel might spin. Keeping its center fixed, change the orientation of the paddlewheel. There will be a preferred orientation, in which the paddlewheel spins the fastest.

We can investigate this situation for any vector field $\vec{\boldsymbol{A}}$. Pick a point P and compute the circulation of $\vec{\boldsymbol{A}}$ around a small loop centered at P. Now change the orientation of the loop and do it again. The result depends on the size of the loop, so we divide by its area. There will be a preferred orientation in which the circulation per unit area will be a maximum. We define the *curl* of $\vec{\boldsymbol{A}}$, written $\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{A}}$, to be the vector whose direction is given by the normal vector to the plane in which the circulation is greatest, and whose magnitude is that circulation divided by the area of the loop, in the limit as the loop shrinks to a point. This construction yields the curl of $\vec{\boldsymbol{A}}$ at P, and we can repeat the process at any point; the curl of $\vec{\boldsymbol{A}}$ is a vector field.

What is the circulation per unit area at the point P in an arbitrary direction? That's just the projection of $\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{A}}$ in the given direction. That is, $(\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{A}}) \cdot \hat{\boldsymbol{u}}$ is the (limiting value of) the circulation per unit area around a loop whose normal vector is $\hat{\boldsymbol{u}}$.

By choosing $\hat{\boldsymbol{u}}$ to be $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$ in turn, we can therefore compute the components of $\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{A}}$ in rectangular coordinates. For further details, see Section 12.9.

12.9 The Definition of Curl

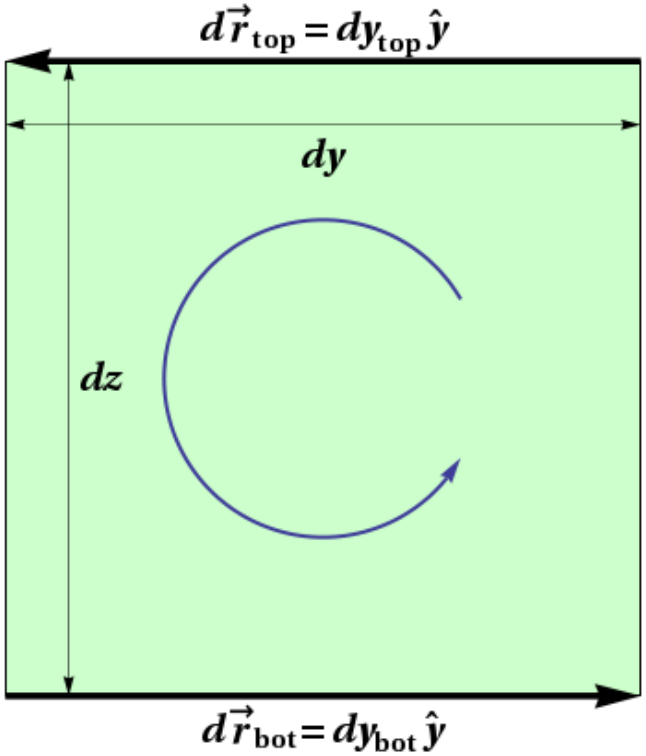


Figure 12.9.1 Computing the horizontal contribution to the circulation around a small rectangular loop.

Consider a small rectangular loop in the yz-plane, with sides parallel to the coordinate axes, as shown Figure 12.9.1. What is the circulation of $\vec{\boldsymbol{A}}$ around this loop?

Consider first the horizontal edges, on each of which $d\vec{\boldsymbol{r}} = dy\,\hat{\boldsymbol{y}}$. However, when computing the circulation of $\vec{\boldsymbol{A}}$ around this loop, we traverse these two edges in opposite directions. In particular, when traversing the loop in the counterclockwise direction, $dy < 0$ on top and $dy > 0$ on the bottom. We would like to compare these two edges, but we have

$$dy_{\text{top}} = -dy_{\text{bot}} \tag{12.9.1}$$

so we conventionally set $dy = dy_{\text{bot}}$, leading to $dy_{\text{top}} = -dy$. [1] Thus,

$$\begin{aligned}\sum_{\text{top+bottom}} \vec{\boldsymbol{A}} \cdot d\vec{\boldsymbol{r}} &= -\vec{\boldsymbol{A}}(z+dz)\cdot\hat{\boldsymbol{y}}\,dy + \vec{\boldsymbol{A}}(z)\cdot\hat{\boldsymbol{y}}\,dy \\ &= -\Big(A_y(z+dz) - A_y(z)\Big)\,dy \\ &= -\frac{A_y(z+dz)-A_y(z)}{dz}\,dy\,dz \\ &= -\frac{\partial A_y}{\partial z}\,dy\,dz \end{aligned} \tag{12.9.2}$$

[1] A similar argument using a finite box would require integrating around the loop, in which case the limits of integration would be equal and opposite for these two edges, leading to an equivalent minus sign when adding the integrals.

where we have multiplied and divided by dz to obtain the surface element $dA = dy\,dz$ in the third step, and used the definition of the derivative in the final step.

Just as with the divergence, in making this argument we are assuming that $\vec{\boldsymbol{A}}$ doesn't change much in the x and y directions, while nonetheless caring about the change in the z direction. We are again subtracting the values at two points separated in the z direction, so we are canceling the zeroth order term in z, and therefore need the next order term. This can be made precise using a multivariable Taylor series expansion.

Repeating this argument for the remaining two sides leads to

$$\begin{aligned}\sum_{\text{sides}} \vec{\boldsymbol{A}} \cdot d\vec{\boldsymbol{r}} &= \vec{\boldsymbol{A}}(y+dy)\cdot\hat{\boldsymbol{z}}\,dz - \vec{\boldsymbol{A}}(y)\cdot\hat{\boldsymbol{z}}\,dz \\ &= \Big(A_z(y+dy) - A_z(y)\Big)\,dz \\ &= \frac{A_z(y+dy)-A_z(y)}{dy}\,dy\,dz \\ &= \frac{\partial A_z}{\partial y}\,dy\,dz\end{aligned}$$

where care must be taken with the signs, which are different from those in (12.9.2). Adding up both expressions, we obtain

$$\text{total } yz\text{-circulation} = \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right) dx\,dy. \tag{12.9.3}$$

Since this expression is proportional to the area of the loop, it approaches zero as the loop shrinks down to a point. The interesting quantity is therefore the ratio of the circulation to area. This ratio is almost the curl, but not quite.

We could have oriented our loop any way we liked. We have a circulation for each orientation, which we can associate with the normal vector to the loop; curl is a vector quantity. Our loop has counterclockwise orientation of the loop as seen from the positive x-axis; we are computing the $\hat{\boldsymbol{x}}$-component of the curl.

Putting this all together, we define the $\hat{\boldsymbol{x}}$-component of the *curl* of a vector field $\vec{\boldsymbol{A}}$ to be

$$\text{curl}(\vec{\boldsymbol{A}})\cdot\hat{\boldsymbol{x}} = \frac{yz\text{-circulation}}{\text{unit area}} = \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}. \tag{12.9.4}$$

The rectangular expression for the full curl now follows by cyclic symmetry, yielding

$$\text{curl}(\vec{\boldsymbol{A}}) = \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right)\hat{\boldsymbol{x}} + \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right)\hat{\boldsymbol{y}} + \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\hat{\boldsymbol{z}} \tag{12.9.5}$$

which is more easily remembered in the form

$$\text{curl}(\vec{\boldsymbol{A}}) = \vec{\boldsymbol{\nabla}}\times\vec{\boldsymbol{A}} = \begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix} \tag{12.9.6}$$

An analogous construction can be used in curvilinear coordinates; the results for spherical and cylindrical coordinates can be found in Appendix B.2, as well as on the inside front of Griffiths' textbook, *Introduction to Electrodynamics*.

12.10 Exploring the Curl

Figure 12.10.1 below shows the relationship between circulation and curl in two dimensions. You can choose the vector field $\vec{v}$ by entering its components v_x and v_y, move the box by dragging its center, and change the size s of the box by moving the slider.

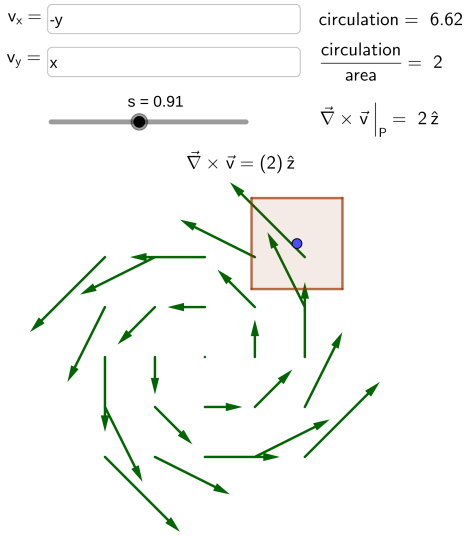


Figure 12.10.1 The relationship between circulation and curl.

Activity 12.10.1 Exploring Curl. Enter the (two-dimensional vector field of your choice into the applet in Figure 12.10.1 by entering its components. Determine the circulation per unit area at several locations by moving the box and adjusting the slider. In each case, compare your result (shown in the applet as $\frac{\text{circulation}}{\text{area}}$) with the computed value of the curl at the center of the box (shown as $\vec{\nabla} \times \vec{v}\big|_P$).

What do you notice?

Hint. Start with vector fields whose components are linear functions of x and y, then try more complicated functions.

12.11 The Curl in Curvilinear Coordinates

Just as with the divergence, similar computations to those in rectangular coordinates can be done using boxes adapted to other coordinate systems. Not surprisingly, this introduces some additional factors of r or s (and $\sin\theta$). You can find expressions for curl in both cylindrical and spherical coordinates in Appendix B.2.

Such formulas for vector derivatives in rectangular, cylindrical, and spherical coordinates, are sufficiently important to the study of electromagnetism that they can, for instance, be found on the inside front cover of Griffiths' textbook, *Introduction to Electrodynamics*.

12.12 Exploring the Curl in Polar Coordinates

Figure 12.12.1 below shows the relationship between circulation and curl using polar coordinates and basis vectors. You can choose the vector field $\vec{v}$ by

entering its components v_r and v_ϕ, move the box by dragging its center, and change the size s of the box by moving the slider.

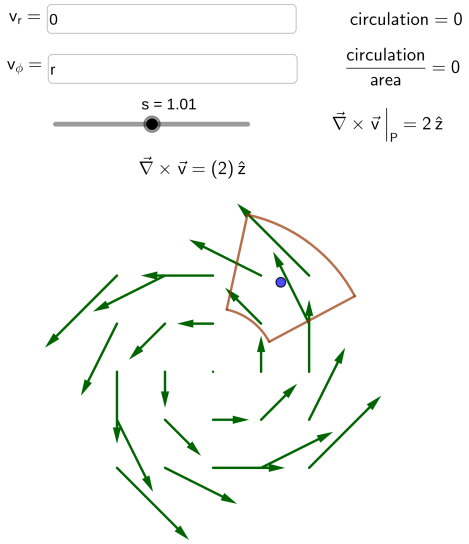


Figure 12.12.1 The relationship between circulation and curl.

Activity 12.12.1 Exploring Curl. Enter the (two-dimensional vector field of your choice into the applet in Figure 12.12.1 by entering its components. Determine the circulation per unit area at several locations by moving the box and adjusting the slider. In each case, compare your result (shown in the applet as $\frac{\text{circulation}}{\text{area}}$) with the computed value of the curl at the center of the box (shown as $\vec{\nabla} \times \vec{v}\big|_P$).

What do you notice?

Hint. Start with vector fields whose components are linear functions of r, then try more complicated functions.

12.13 Visualizing Curl

Recall that

$$(\vec{\nabla} \times \vec{F}) \cdot \hat{n} \approx \frac{\oint \vec{F} \cdot d\vec{r}}{\text{area of loop}} = \frac{\text{(oriented) circulation}}{\text{unit area}} \tag{12.13.1}$$

so that the (orthogonal component of the) curl measures how much a vector field "goes around" a loop.

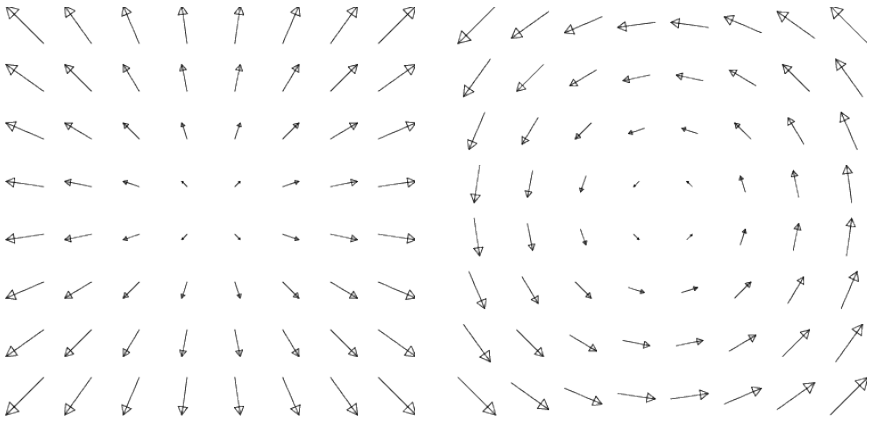


Figure 12.13.1 Two vector fields.

Can we use these ideas to investigate graphically the curl of a given vector field?

Activity 12.13.1 The Geometry of Curl. Consider the two vector fields in Figure 12.13.1. In each case, can you find the ($\hat{\boldsymbol{z}}$-component of the) curl?

Hint. A natural place to start is at the origin. So draw a small box around the origin, as shown in Figure 12.13.2. Is there circulation around the loop?

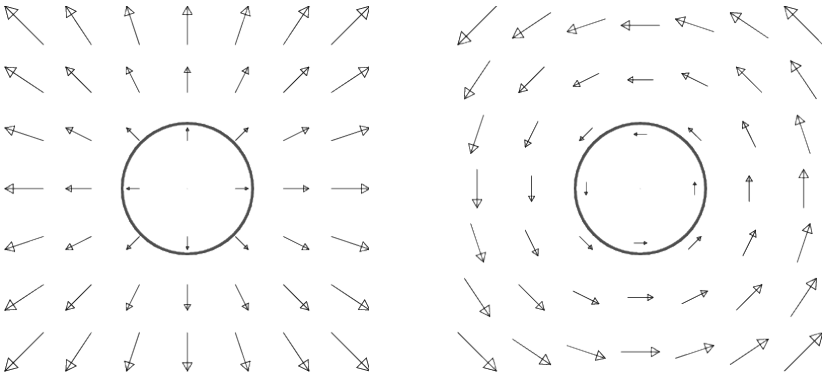


Figure 12.13.2 The same two vector fields, with loops at the origin.

The figures above help us determine the curl *at the origin*, but not elsewhere. The curl is a vector field, which can vary from point to point. We therefore need to examine loops which are *not* at the origin. It is useful to adapt the shape of our loop to the vector field under consideration. Both of our vector fields are better adapted to polar coordinates than to rectangular coordinates, so we use polar boxes. Can you determine the ($\hat{\boldsymbol{z}}$-component of the) curl using the loops in Figure 12.13.3? Imagine trying to do the same thing with a rectangular loop, or even a circular loop.

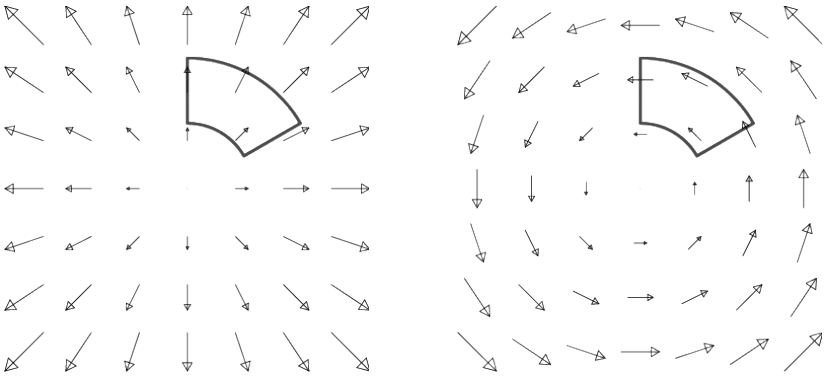


Figure 12.13.3 The same two vector fields, with loops not at the origin.

Finally, it is important to realize that not all vector fields which go around the origin have curl. The example in Figure 12.13.4 demonstrate this important principle; it has no curl away from the origin. This figure represents a solution of Maxwell's equations for electromagnetism, and describes the magnetic field due to an infinite current-carrying wire (with current coming out of the page at the origin).

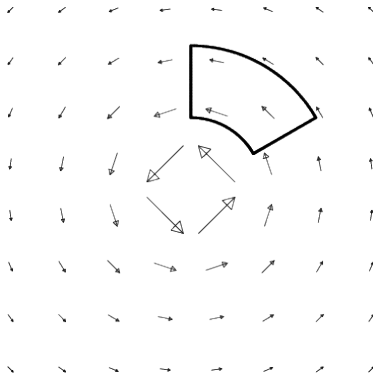


Figure 12.13.4 One more vector field.

12.14 Stokes' Theorem

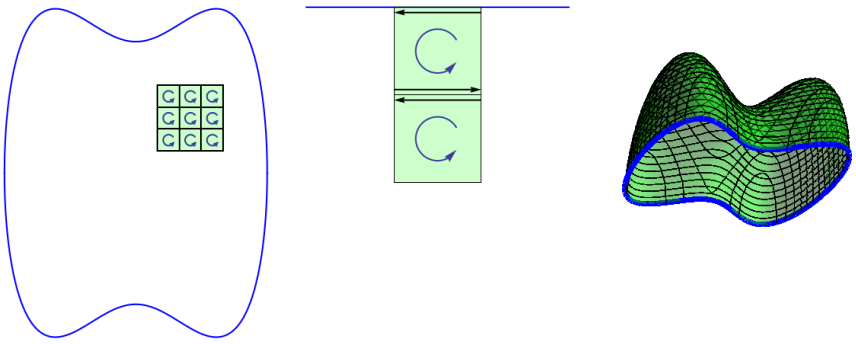


Figure 12.14.1 The geometry of Stokes' Theorem.

The total circulation of the magnetic field around a small loop is given by

$$\text{circulation} = \sum_{\text{box}} \vec{\boldsymbol{B}} \cdot d\vec{\boldsymbol{r}} = (\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{B}}) \cdot d\vec{\boldsymbol{A}}$$

where $d\vec{\boldsymbol{A}} = \hat{\boldsymbol{n}}\, dA$, where $\hat{\boldsymbol{n}}$ is perpendicular to the (filled in) loop. But any surface can be filled with such loops, as shown in the first diagram in Figure 12.7.1. Furthermore, the circulation around the edge of the surface is just the sum of the circulations around each of the smaller loops, since the circulation through any common side will be zero (because adjacent loops have opposite notions of "around"), as indicated schematically in the second diagram in Figure 12.7.1. Thus, the total circulation around any loop is given by

$$\oint_{\text{loop}} \vec{\boldsymbol{B}} \cdot d\vec{\boldsymbol{r}} = \int_{\text{inside}} (\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{B}}) \cdot d\vec{\boldsymbol{A}}$$

This is *Stokes' Theorem*.

There is no need for the "inside" of the loop to be planar. [1] Consider the surface shown in the third diagram in Figure 12.7.1, which has the same boundary as the original loop. The circulation around interior loops cancels just as before, and Stokes' Theorem holds without modification. We like to describe such surfaces as "butterfly nets", whose rim is the original loop. Butterfly nets should be able to catch butterflies! In other words, they need an opening, and a net. [2]

The orientations used in the two integrals in Stokes' Theorem must be compatible. This is easy if the loop lies in the xy-plane: Choose the circulation *counterclockwise* and the flux *upward*. More generally, for any loop which is more-or-less planar, the circulation should be counterclockwise when looking at the loop from "above", that is, *from* the direction in which the flux is being taken. (So you're really looking in the direction of *negative* flux.) An easy way to remember this is to take the flux *up* and the circulation *counterclockwise when seen from above*, with obvious modifications should the loop be sideways.

But what if the loop is not planar? What about a cylinder which is closed at one end? There are several strategies which can be used to obtain compatible orientations.

- *Gears:* Break up the surface into small loops, which can be thought of as small gears. Choose an orientation of the surface, and look at the surface from "above". As the gears turn counterclockwise, the edge of the surface also turns; use that orienation to compute the circulation.

- *Toothpicks:* Think of the surface as a rubber sheet. Move the rubber sheet so that it is taut across the loop. Choose a compatible orientation using the "up" and "counterclockwise" rule. Now imagine putting toothpicks in the surface on the "up" side only, and move the rubber sheet back to the original position. The direction of the toothpicks gives you the compatible orientation of the surface.

- *Left-Hand Rule:* Walk around the edge of the surface, with your head up. That is, face in the direction $\hat{\boldsymbol{T}}$, with your head in the direction $\hat{\boldsymbol{n}}$ (where $d\vec{\boldsymbol{r}} = \hat{\boldsymbol{T}}\, ds$ and $d\vec{\boldsymbol{A}} = \hat{\boldsymbol{n}}\, dA$). In a compatible orientation, your *left* hand should point along the surface; if it doesn't, turn around (or stand on your head, but not both).

[1] There is also no need for the loop itself to be planar.

[2] Can you imagine a butterfly net with more than one opening? Can you work out the form of Stokes' Theorem on such a net?

12.15 Second derivatives

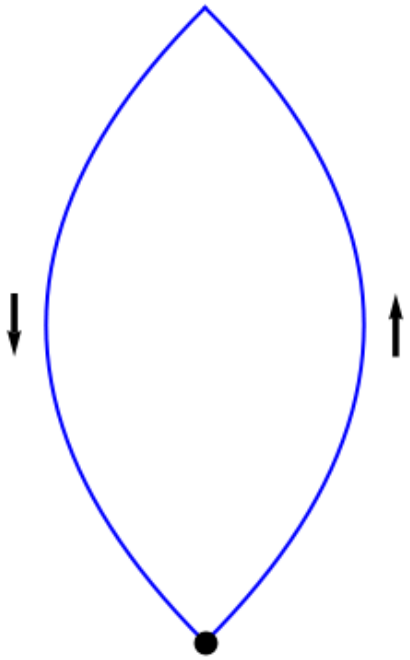


Figure 12.15.1 A closed path.

A conservative vector field is the gradient of some function, for example

$$\vec{\boldsymbol{E}} = -\vec{\boldsymbol{\nabla}} V$$

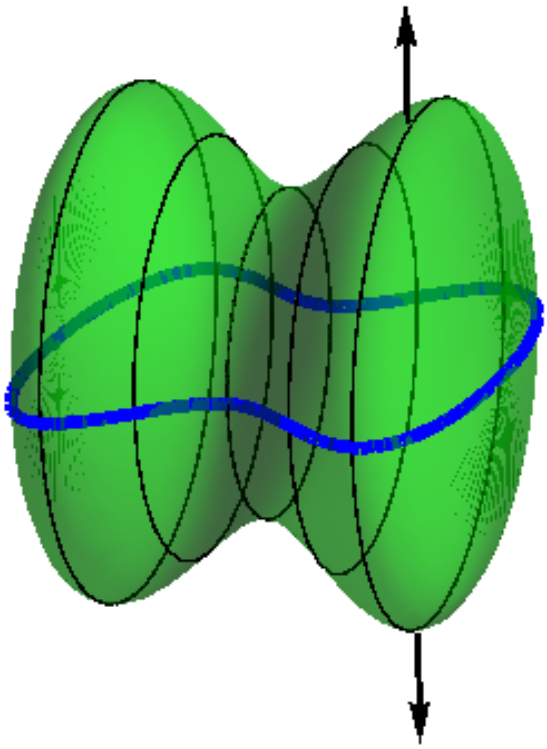
But integrals of conservative vector fields are independent of path, so that evaluating the integral along two different paths between the same two points yields the same answer, as illustrated in [2]. Combining two such paths into a closed loop changes the orientation of one path, as shown in Figure 12.15.1, and the integrals now cancel; the integral of $\vec{\boldsymbol{\nabla}} V$ around any closed loop vanishes. Using Stokes' Theorem, we therefore obtain

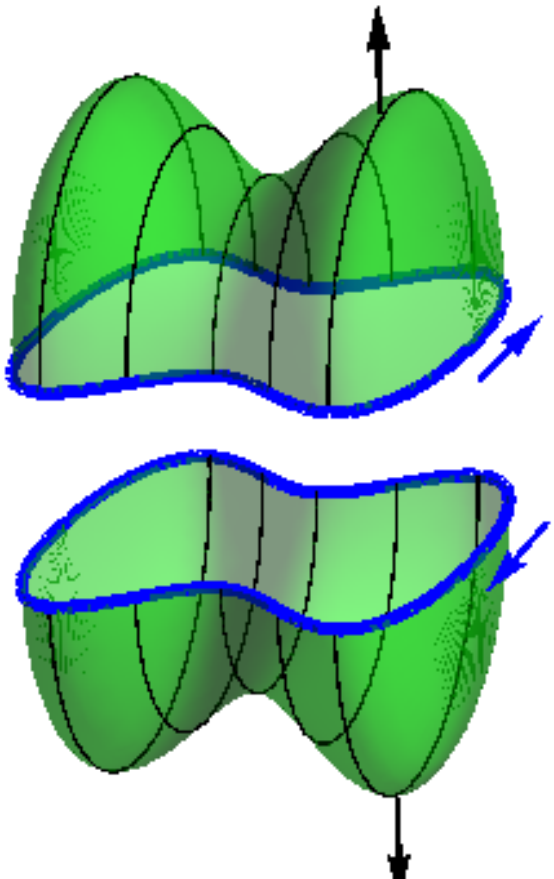
$$\int_{\text{inside}} (\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{\nabla}} V) \cdot d\vec{\boldsymbol{A}} = \oint_{\text{loop}} \vec{\boldsymbol{\nabla}} V \cdot d\vec{\boldsymbol{r}} = 0. \tag{12.15.1}$$

Equivalently, the Master Formula tells us how to evaluate the left-hand side of (12.15.1), namely by evaluating the potential at the endpoints. Since both endpoints are the same, the integral must be zero. But since the left-hand side must vanish for *any* closed curve, the integrand must be identically zero. We have proved that

$$\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{\nabla}} V = \vec{\boldsymbol{0}}$$

for *any* function V.





A similar argument can be used to show that

$$\vec{\boldsymbol{\nabla}} \cdot (\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{F}}) = 0$$

for *any* vector field $\vec{\boldsymbol{F}}$. Consider a closed surface. Cut it in half along some closed curve, as shown in the first diagram in Figure 12.15.2. Then each piece of the surface is a butterfly net with the same rim, as shown in the second diagram in Figure 12.15.2 (with the pieces separated for clarity). Applying Stokes' Theorem to each piece leads to the conclusion that the flux of the curl of $\vec{\boldsymbol{F}}$ *upward* through each piece must be the same, so that the flux *up* through the top cancels the flux *downward* through the bottom. This cancellation forces the flux of the curl of $\vec{\boldsymbol{F}}$ *outward* through the entire surface to vanish. Using the Divergence Theorem, we get

$$\int\limits_{\text{inside}} \vec{\boldsymbol{\nabla}} \cdot (\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{F}})\, d\tau = \int\limits_{\text{surface}} (\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{F}}) \cdot d\vec{\boldsymbol{A}} = 0$$

This argument shows that the first integral is zero over *any* volume, forcing the integrand to vanish, as claimed.

The above identities can also be derived by direct computation, most easily done in rectangular coordinates. For instance, when calculating the curl of $\vec{\boldsymbol{\nabla}} V$, each component will contain mixed second-order partial derivatives of V, for example:

$$\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{\nabla}} V = \ldots + \left(\frac{\partial}{\partial x} \frac{\partial V}{\partial y} - \frac{\partial}{\partial y} \frac{\partial V}{\partial x} \right) \hat{\boldsymbol{z}}$$

But partial derivatives can be taken in any order, so the derivatives above cancel, thus proving the identity. Similar second-order derivatives arise when computing the divergence of $\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{A}}$, establishing the other identity.

12.16 The Laplacian

One second derivative, the divergence of the gradient, occurs so often it has its own name and notation. It is called the *Laplacian* of the function V, and is written in any of the forms

$$\triangle V = \nabla^2 V = \vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{\nabla}} V.$$

In rectangular coordinates, it is easy to compute

$$\triangle V = \vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{\nabla}} V = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2}.$$

The simplest homogeneous partial differential equation involving the Laplacian

$$\nabla^2 V = 0 \tag{12.16.1}$$

is called Laplace's equation. The inhomgeneous version

$$\nabla^2 V = f(\vec{\boldsymbol{r}}) \tag{12.16.2}$$

is known as Poisson's equation. There are many important techniques for solving these equations that are beyond the scope of this text.

Chapter 13

Power Series

13.1 Definition of Power Series

Form of Power Series. Most functions can be represented as a **power series**, whose general form is given by:

$$\begin{aligned} f(z) &= \sum_{n=0}^{\infty} c_n (z-a)^n \\ &= c_0 + c_1(z-a) + c_2(z-a)^2 + c_3(z-a)^3 + \dots \end{aligned} \tag{13.1.1}$$

In this equation, for a given function $f(z)$, a is a constant that you get to choose and the c_n's are constants that will be different if you change a.

Notation 13.1.1 Power Series. In Equation (13.1.1), z is the independent variable of the function, a represents the point "around" which the function is being expanded, each of the constants c_n is called the *coefficient* of the nth term, and the entire nth term, i.e. $c_n(z-a)^n$, is called the nth *order* term. For further information about the geometric meaning of these new vocabulary words, see Section 13.4.

Informal theorem: A deep mathematical theorem guarantees that for each sufficiently smooth function $f(z)$ and point a, the coefficients c_n are unique. You can always find the coefficients, using the general method in Section 13.2. However, you should also gradually accumulate as many short-cut strategies as you can for finding these coefficients. The theorems in Section 13.10 will help.

13.2 Calculating Power Series Coefficients

Derivation of the Formula for the Coefficients of a Power Series. One way of finding the coefficients is using Taylor's theorem, derived as follows:

We evaluate both sides of equation (13.1.1) at the point $z = a$, to obtain:

$$f(a) = c_0 + c_1(a-a) + c_2(a-a)^2 + c_3(a-a)^3 + \dots \tag{13.2.1}$$

Since all of the terms, except the first, on the right hand side of (13.2.1) are zero, the equation simplifies to:

$$c_0 = f(a) \tag{13.2.2}$$

To find the next coefficient, c_1, we first differentiate (13.1.1)

$$f'(z) = c_1 + 2c_2(z-a) + 3c_3(z-a)^2 + \dots \tag{13.2.3}$$

We then evaluate (13.2.3) at $z = a$ to obtain

$$c_1 = f'(a) \tag{13.2.4}$$

We continue to differentiate (13.2.3) and then evaluate at $z = a$, reordering the equation as necessary

$$\begin{aligned} f''(z) &= 2c_2 + (3)(2)(z-a) + \dots \\ c_2 &= \frac{1}{2} f''(a) \end{aligned}$$

The nth coefficient is given by

$$c_n = \frac{1}{n!} \frac{d^n}{dz^n} f(z)\Big|_{z=a} \tag{13.2.5}$$

$$= \frac{1}{n!} f^{(n)}(a) \tag{13.2.6}$$

where the last line is just a common notation for the previous line.

Notation. i.e. the symbol $f^{(n)}$ means to take n derivatives of f.

Make sure to evaluate the derivatives at $z = a$ only *after* you have taken the required number of derivatives.

By plugging these values of the coefficients into Equation (13.1.1), we obtain the following form of the power series:

$$f(z) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n}{dz^n} f(a)\,(z-a)^n \tag{13.2.7}$$

Sensemaking 13.2.1 Why is there a factor of $1/n!$ in (13.2.6), the expression for the nth coefficient?

To check your understanding of this section you should complete the following activity.

Activity 13.2.2

1. Find the first five nonzero coefficients for $\sin(\theta)$ expanded around the origin.

2. Write out a series approximation, correct to fourth order, for $\sin(\theta)$ expanded around the origin.

$$\sin(\theta) =$$

3. Find the first four nonzero coefficients for $\sin(\theta)$ expanded around $\theta_0 = \frac{\pi}{6}$.

4. Write out a series approximation, correct to fourth order, for $\sin(\theta)$ expanded around $\theta_0 = \frac{\pi}{6}$.

$$\sin(\theta) =$$

Hint. Some important observations are given below:

1. Pay attention to the name of the independent variable. The equation for the coefficients is given in terms of the variable z. What is the independent variable in $\sin\theta$?

2. Commonly, but not always, there are an infinite number of terms in a power series expansion. Unless you can find a general expression for the coefficients, it will take you an infinite amount of time to find all of them. In practice, one usually stops at some stage. Some language for this: "find the first four non-zero terms" means find the coefficients for the four lowest powers of the independent variable, continuing until you have four that are not zero; "find the expansion correct to fourth order" means find the coefficients for all of the low powers of the independent variable, up to and including the fourth power.

3. If you are asked to find the power series expansion around $z = a$, then you must plug the number a into all of the derivatives.

4. Your final answer for a power series expansion should be of the form

$$f(z) = c_0 + c_1(z-a) + c_2(z-a)^2 + c_3(z-a)^3 + \ldots \tag{13.2.8}$$

or

$$f(z) \approx c_0 + c_1(z-a) + c_2(z-a)^2 + c_3(z-a)^3 \tag{13.2.9}$$

where you have plugged in numbers for all of the c_n and for a. Use the first form of the equation, with an equals sign, if you include the symbol $\ldots$ to remind yourself that there are (an infinite number of) terms that you have not written down. Use the second form of the equation, with an approximately equals sign, if you have truncated the series, leaving out (a possibly infinite number of) terms.

13.3 Visualization of Power Series Approximations

In the activities in this section you have the opportunity to explore what it means to approximate a given function with a power series expansion, truncated at different orders.

Activity 13.3.1 Visualization of Power Series Approximations. In the *Sage* code below or this *Mathematica* notebook[1], you will begin with the function $f(\theta) = \sin\theta$. Look at the first few terms of its power series. Using the coefficients that you found in Activity 13.2.2, you can plot both the function $\sin\theta$ and its various approximations found by truncating the power series, first after one non-zero term, then after two non-zero terms, etc. Write down as many features as you can of these approximations. In particular, answer the following questions:

1. For what values of θ is the approximation a "good" one? What is the definition of "good"?

2. Does the range of good values of θ depend on the order of the approximation? If so, how?

3. A function $f(z)$ is called *symmetric* if the graph of the function for negative values of its argument is the mirror reflection (with the vertical axis acting as mirror) of the graph of the function for positive values of its argument, i.e. if $f(-z) = f(z)$. Similarly, a function is called *antisymmetric* if the graph of the function for negative values of its argument is the negative of the mirror reflection (with the vertical axis acting as mirror) of the graph of the function for positive values of its argument, i.e. if $f(-z) = -f(z)$.

Is the function $f(z)$ symmetric, antisymmetric, or neither? What about the various terms in the power series expansion?

Answer. Notice that if you truncate a power series, then you are looking at a polynomial whose dominant term (i.e. highest power) is the highest term that you kept in the power series. Since $\sin\theta$ is bounded for large θ and a polynomial in θ is not bounded, the first few terms of the power series will be a terrible approximation for the function if $|\theta|$ is large enough. However, as you keep more and more terms in the series, the truncated series is a better and better approximation for the function for a larger and larger range of values of θ.

This computer algebra worksheet began by approximating $\sin\theta$ by θ near the origin. This small angle approximation may be familiar to you from your study of the motion of a pendulum. Higher order terms add more higher order polynomials and therefore add more "bumps" to the curve; the graph of $\sin\theta$ has infinitely many bumps. It is remarkable that the power series for $\sin\theta$ converges for all values of θ.

You can see from the graphs that all even positive integer powers of z are symmetric; all odd positive integer powers are antisymmetric. Since the function $f(\theta) = \sin\theta$ is an odd function of θ, only the odd powers of θ appear in the power series expansion. You can see this antisymmetry in Figure Figure 13.3.1.

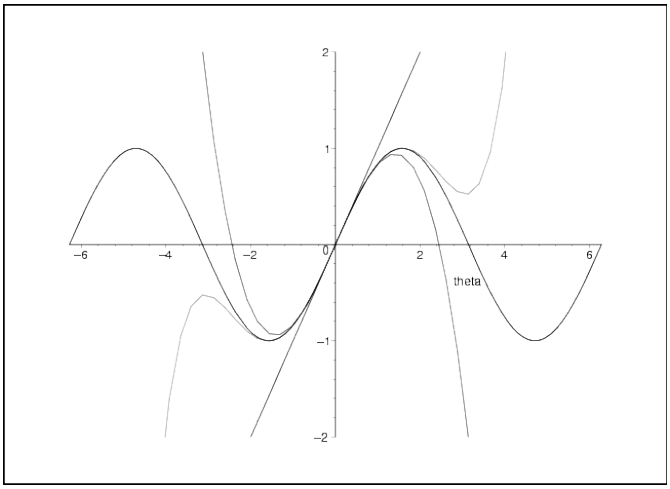


Figure 13.3.1 The function $\sin\theta$ and three approximations formed from truncating the power series after the first, second, and third non-zero terms (i.e. at the first, third, and fifth order.)

The *Sage* code below allows you to plot both a function $f(x)$ (entered at line 2) and your choice of polynomial approximation $p(x)$ (entered at line 3). The defaults are $f(x) = \sin x$ and $p(x) = x$ (the first-order term). You can change these defaults to look at any reasonable function and any order of approximation.

```
x=var('x')
f(x)=sin(x)
p(x)=x
F=plot(f(x),(x,-5,5))
P=plot(p(x),(x,-5,5),ymin=-2,ymax=2,color=Color('purple'))
F+P
```

[1] `math/vfpowerapprox.nb`

See Figure 13.3.1.

Activity 13.3.2 Power Series Expansions around Points Other than the Origin. You can (and should) also alter the same Sage or Mathematica code to make a power series approximation that fits a function well somewhere other than at the origin by writing the power series expanded "around" some other point such as $\theta = \frac{\pi}{6}$.

13.4 Discussion of Approximations using Power Series

Why should you care about power series? One reason is because they allow us to approximate functions *at a point* to any desired accuracy.

For instance, consider the function $h(x) = -1 - 2x + x^2$. Draw its graph.

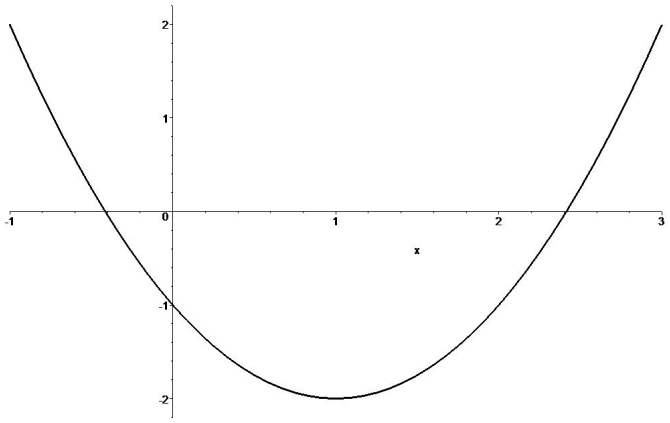


Figure 13.4.1 The graph of the polynomial $h(x) = -1 - 2x + x^2$.

Notice that we have chosen a particularly simple function for this example, a polynomial. Just by looking at it; you can see that the function already has the form of a power series with only three nonzero terms. Its power series, expanded around the origin, is just the algebraic expression for the function itself. Obviously, there is no reason for you to approximate a function this simple. We are using this simple example so that you can think about the separate terms quickly and easily in your head. In Section 13.2 and Section 13.3 you have the opportunity to work with the power series for $\sin\theta$, which has an infinite number of terms. You will have many chances to see why power series approximations are useful for more complicated functions later in this text.

At the origin $x = 0$, the value of the function is -1. So, the zeroth order approximation is just the constant function -1. It agrees with the value of the function exactly at $x = 0$, but otherwise is a pretty lousy approximation, see Figure 13.4.2. The slope of this graph at $x = 0$ is given by the derivative, namely 2. The linear approximation at the origin to this function is therefore the straight line $y = -1 - 2x$. Where is this linear approximation for this function a "good" approximation?

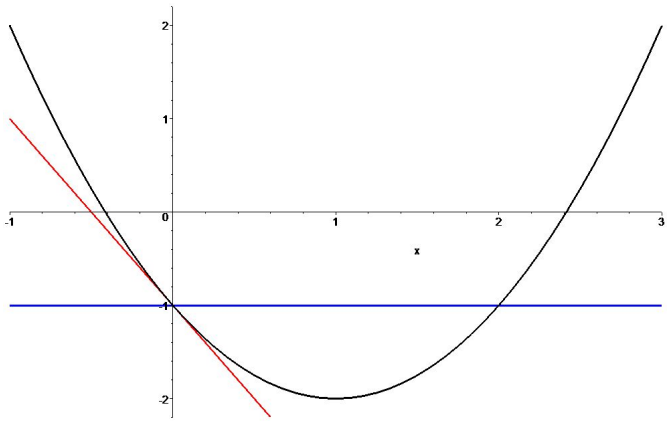


Figure 13.4.2 The graph of the polynomial $h(x) = -1 - 2x + x^2$ (black) together with its zeroth order (constant) approximation at the origin (blue) and its first order (linear) approximation at the origin (red).

The approximation that we found above, which was a first order series expansion around $x = 0$ isn't a very good approximation near $x = 1$. We can find a better approximation if we choose to expand around another point, say $x = 1$, see Figure 13.4.3. The expansion of h around 1 has just two terms, namely $h(x) = -2 + (x - 1)^2$. The absence of a linear term in this expansion tells us that the graph is horizontal at $x = 1$.

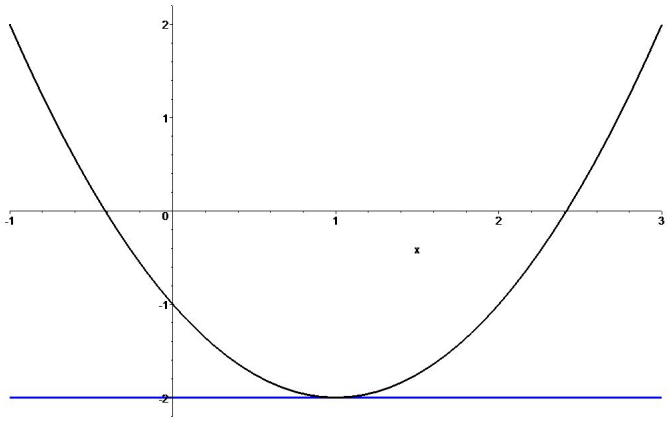


Figure 13.4.3 The graph of the polynomial $h(x) = -1 - 2x + x^2$ (black) together with its zeroth order (and linear) approximation at $x = 1$ (blue).

You can explore power series approximations for yourself using the applet in Section 13.5

13.5 Using Technology to Explore Power Series Approximations

The applet below in Figure 13.5.1 shows power series expansions of different orders for any (reasonable) function, at different points, corresponding to the data entered. You can change what function you are looking at in the box near the top of the graph.

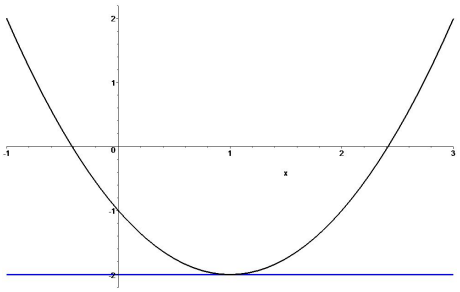


Figure 13.5.1 Power series approximations.

13.6 Guessing Power Series from Graphs

Activity 13.6.1 Guessing Power Series Coefficients. In Figure 13.6.1 below, use the sliders to match the given function (shown in green) exactly. Use only graphical reasoning.

When you are done, make a note of any relationship you see between the values of the coefficients and the shape of the graph.

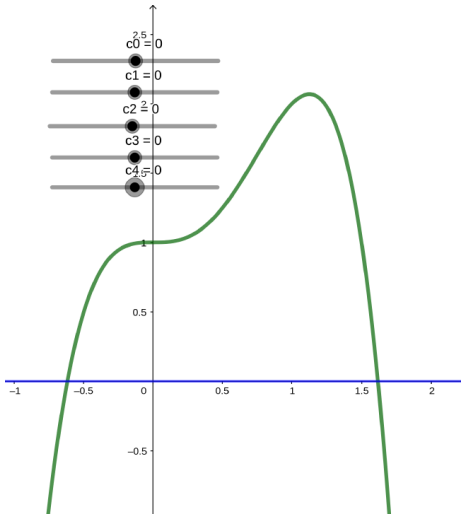


Figure 13.6.1 An applet for manipulating the individual power series coefficients.

Hint. Only three of the sliders need to be set to nonzero values.

13.7 Common Power Series

The following power series for common functions are used so often in approximations in physics, that you should make the extra effort to memorize the first few terms of each one.

The symbol $\forall$ means "for all"

$$\begin{aligned}\sin(z) &= z - \frac{z^3}{3!} + \frac{z^5}{5!} - \frac{z^7}{7!} + \dots \\ &= \sum_{n=0}^{\infty} (-1)^n \frac{z^{2n+1}}{(2n+1)!} \qquad \text{valid } \forall z\end{aligned}$$

$$\begin{aligned}
\cos(z) &= 1 - \frac{z^2}{2!} + \frac{z^4}{4!} - \frac{z^6}{6!} + \dots \\
&= \sum_{n=0}^{\infty} (-1)^n \frac{z^{2n}}{(2n)!} && \text{valid } \forall z \\
e^z &= 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \frac{z^4}{4!} + \dots \\
&= \sum_{n=0}^{\infty} \frac{z^n}{n!} && \text{valid } \forall z \\
\ln(1+z) &= z - \frac{z^2}{2} + \frac{z^3}{3} - \frac{z^4}{4} + \dots \\
&= \sum_{n=1}^{\infty} (-1)^{n+1} \frac{z^n}{n} && \text{valid for } |z| < 1 \\
(1+z)^p &= 1 + pz + \frac{p(p-1)}{2!} z^2 + \frac{p(p-1)(p-2)}{3!} z^3 + \dots \\
&= \sum_{n=0}^{\infty} \frac{p!}{n!(p-n)!} z^n && \text{valid for } |z| < 1
\end{aligned}$$

The factorial function can be extended to the domain of all complex numbers, except the negative integers. See "gamma function" in any advanced mathematical methods text.

The last example, called a binomial expansion is valid even when p is not a positive integer. You may not know the meaning of $p!$ in these cases, but it does have a definition. If necessary, just use the first line of the power series for $(1+z)^p$ instead of the second line.

13.8 Dimensions in Power Series

When we consider a power series expansion of a special function such as

$$\sin z = z - \frac{1}{3!} z^3 + \frac{1}{5!} z^5 + \dots \tag{13.8.1}$$

we can notice an interesting fact. If the variable z were to have any kind of dimensions (e.g. length, L) then the power series expansion of that special function would add together terms with different dimensions (L, L^3, L^5, etc.). Since this is impossible, it implies that the argument of such special functions must always be dimensionless. This fact provides a quick check in many long algebraic manipulations. Look for expressions like $\sin \frac{x}{a}$ rather than $\sin x$, where a is a physical parameter with the same dimensions as x.

Sensemaking 13.8.1 Logarithms (Optional, Advanced). Is the logarithm function an exception to this rule?

Answer. Consider the logarithm rule

$$\ln(ab) = \ln(a) + \ln(b) \tag{13.8.2}$$

if a has non-trivial dimensions, but ab is dimensionless. Then the power series expansion of the left-hand side of (13.8.2) will be a sum of dimensionless terms, as expected, but the power series expansion of the right-hand side of (13.8.2) might appear to have terms of different dimensions. The resolution is that the expansion parameters a and b are really $\frac{a}{1}$ and $\frac{b}{1}$, where the factors of 1 have the appropriate dimensions to make the expansion parameters dimensionless.

13.9 Convergence of Power Series

Most often, we use a power series for real values of its independent variable, but they work perfectly well for complex variables. It is actually easier to study the set of values for which a power series is valid, called its *region or circle of convergence*, if we think of it as a function of a complex variable. If a function has a power series expansion around some point a, then the circle of convergence extends to the nearest point at which the function is not analytic. (Briefly, a function which is not analytic is singular in some way. A function is certainly not analytic at any point at which its value becomes infinite or at a branch point of a root.) For example, the function $\frac{1}{z^2+1}$ seems perfectly well-behaved if z is real, but blows up if $z = \pm i$. If we expand this function in a power series around $z = 0$, using the binomial expansion in Section 13.7, the resulting series is valid for $|z| \leq 1$, i.e. inside a circle with radius 1.

13.10 Theorems about Power Series

Theorem 13.10.1 Uniqueness of Power Series. *The power series of a function, if it exits, is unique, i.e. there is at most one power series of the form $\sum_{n=0}^{\infty} c_n(z-a)^n$ which converges to a given function within a circle of convergence centered at a. We call this a power series "expanded around a".*

This theorem is an open invitation to collect a bag of cute tricks. It doesn't matter how you find a series for a function, once you have it, it is *the* series. The rest of the theorems in this section should be in your bag of cute tricks. Scientists use these theorems, rather that the method in Section 13.2 to find series expansions whenever possible. We give these theorems without proof, but include one or more examples of how each is used, in practice. It is worth taking the time to work carefully through each of these short examples.

Theorem 13.10.2 Differentiation and Integration of Power Series. *A power series may be differentiated or integrated term by term. The resulting series converges to the derivative or integral of the function represented by the original series within the same circle of convergence as the original series.*

Example 13.10.3

$$\sin z = \sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{(2n+1)!} \qquad \forall z$$

$$\cos z = \frac{d}{dz}\sin z = \sum_{n=0}^{\infty} \frac{(-1)^n (2n+1) z^{2n}}{(2n+1)!}$$

$$= \sum_{n=0}^{\infty} \frac{(-1)^n z^{2n}}{(2n)!} \qquad \forall z$$

□

Theorem 13.10.4 Substitution in Power Series. *One series may be substituted into another provided that the values of the substituted series are inside the circle of convergence of the other series.*

Example 13.10.5

$$\frac{1}{1+z} = 1 - z + z^2 - z^3 + \cdots = \sum_{n=0}^{\infty} (-z)^n \qquad |z| < 1$$

$$\begin{aligned}\frac{1}{1+\sin z} &= 1 - \sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{(2n+1)!} + \left(\sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{(2n+1)!}\right)^2 \\ &\quad - \left(\sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{(2n+1)!}\right)^3 + \dots \\ &= 1 - z + z^2 + \left(\frac{1}{3!} - 1\right) z^3 + \dots \qquad |\sin z| < 1\end{aligned}$$

What happens if you try this same trick to find a power series for $1/(1+\cos z)$? Why? □

Example 13.10.6

$$z - \frac{\pi}{2} = z - \frac{\pi}{2} \qquad \forall z$$

Note: This is a very short power series with just two non-zero terms.

$$\begin{aligned}\cos(z) &= -\sin(z - \frac{\pi}{2}) \\ &= \sum_{n=0}^{\infty} \frac{(-1)^{n+1}(z - \frac{\pi}{2})^{2n+1}}{(2n+1)!} \qquad \forall z\end{aligned}$$

Note: Starting with a power series for $\sin(z)$ expanded around $z = 0$, we have obtained a power series for $\cos(z)$ expanded around $z = \frac{\pi}{2}$. □

Theorem 13.10.7 Adding, Subtracting, and Multiplying Power Series. *Two power series of like powers may be added, subtracted, or multiplied. The resulting series converges at least within the common circle of convergence.*

Example 13.10.8

$$\begin{aligned}\frac{2}{1-z^2} &= \frac{1}{1+z} + \frac{1}{1-z} \\ &= (1 - z + z^2 - z^3 + \dots) + (1 + z + z^2 + z^3 + \dots) \\ &= 2(1 + z^2 + z^4 + \dots) \qquad |z| < 1\end{aligned}$$

Compare this to the result you would get using the previous theorem. Which method is faster? □

Example 13.10.9

$$\begin{aligned}\frac{\sin z}{1+z} &= \left(z - \frac{z^3}{3!} + \frac{z^5}{5!} + \dots\right)\left(1 - z + z^2 - z^3 + z^4 - z^5\right) \\ &= z - z^2 + \left(-\frac{1}{3!} + 1\right) z^3 + \left(\frac{1}{3!} - 1\right) z^4 \\ &\quad + \left(\frac{1}{5!} - \frac{1}{3!} + 1\right) z^5 + \dots \qquad |z| < 1\end{aligned}$$

Compare this series to the series for the function $1 - \frac{1}{1+\sin(z)}$ in Example 13.10.5. What can you conclude about the wisdom of assuming two series are the same if their first three terms are identical? □

Theorem 13.10.10 Dividing Power Series. *Two power series expanded around the same point may be divided. If the leading term(s) of the denominator series is not zero, or if the zero(s) is canceled by the numerator, then the resulting series converges within some circle. If the radius of convergence of the*

numerator and denominator series are r_1 and r_2, respectively, and the distance from the origin of the circles to the nearest zero of the denominator series is s, then the quotient series converges at least inside the smallest of the three circles of radii r_1, r_2, and s.

Example 13.10.11 Try the previous example $\sin z/(1+z)$ using synthetic division, instead. Is this method easier or harder? Imagine what you would do if the denominator were a power series with an infinite number of non-zero terms. □

Theorem 13.10.12 Power Series Around Points Other than Zero. *The series expansions for most functions recorded in books are expansions around the point $z = 0$. To expand around a point $a \neq 0$ write every z which appears in the function as $(z-a)+a$, simplify creatively, and use Theorem 13.10.4.*

Example 13.10.13 Expand $\sin z$ around $z = \pi$.

$$\begin{aligned}
\sin z &= \sin[(z-\pi)+\pi] \\
&= \sin(z-\pi)\cos\pi + \cos(z-\pi)\sin\pi \\
&= -\sin(z-\pi) \\
&= -\sum_{n=0}^{\infty} \frac{(-1)^n (z-\pi)^{2n+1}}{(2n+1)!} \qquad \forall z
\end{aligned}$$

□

Chapter 14

Vector Spaces

14.1 Definition of a Vector Space

In this section, we give the formal definitions of a vector space and list some examples.

Definition 14.1.1 Vector Space. A set of objects (vectors) $\{\vec{u}, \vec{v}, \vec{w}, \dots\}$ is said to form a **linear vector space over the field of scalars** $\{\lambda, \mu, \dots\}$ (e.g. real numbers or complex numbers) if:

1. the set is closed, commutative, and associative under (vector) addition;
2. the set is closed, associative, and distributive under multiplication by a scalar;
3. there exists a **zero vector** $\vec{0}$ that leaves other vectors unchanged under addition;
4. multiplication by the scalar identity 1 leaves the vector unchanged;
5. every vector $\vec{v}$ have a corresponding **negative vector** $-\vec{v}$ such that $\vec{v} + (-\vec{v}) = \vec{\mathbf{0}}$;

$\Diamond$

The trick here is not only to identify the set of objects that are in the vector space, but also what is meant by *addition of vectors* and *scalar multiplication.*

Some examples of vector spaces are:

1. Forces on a point particle that can move in a plane (i.e. arrows in 2-D).
2. Forces on a point particle that can move in space (i.e. arrows in 3-D). Notice that arrows in 2-D and arrows in 3-D are *different* vector spaces.
3. $m \times n$ matrices for fixed m and n.
4. Sufficiently smooth functions on the interval $0 \leq x \leq L$ that go to zero at $x = 0$ and $x = L$, as in quantum particle-in-a-box.
5. Periodic functions with a fixed period, e.g. Fourier Series.

Activity 14.1.1 Definition of addition for example vector spaces. For each of the example vector spaces above, state what is meant by the sum of two vectors.

Answer. For arrows, addition means the parallelogram rule. For matrices, addition means component by component, which is equivalent to the parallel-

ogram rule if the matrices happen to be columns. For functions, addition is pointwise addition of functions.

14.2 Definition and Properties of an Inner Product

We have already discussed the concept of a dot product Section 3.6 or inner product Section 3.7 in the simplest examples of vector spaces when we can think of the vectors as either arrows in space or as columns of real or complex numbers. In this section, we generalize the concept of inner product to ANY vector space.

Definition 14.2.1 Inner Product. An **inner product** $\langle \vec{u} | \vec{v} \rangle$ is a generalization of the dot product with the following properties:

$$\langle \vec{u} | \vec{v} \rangle = \langle \vec{v} | \vec{u} \rangle^* \tag{14.2.1}$$

$$\langle \vec{u} | \lambda \vec{v} + \mu \vec{w} \rangle = \lambda \langle \vec{u} | \vec{v} \rangle + \mu \langle \vec{u} | \vec{w} \rangle \tag{14.2.2}$$

Like the dot product, the inner product is always a rule that takes two vectors as inputs and the output is a scalar (often a complex number). ◊

While most vector spaces in physics have a natural and obvious inner product, the existence of an inner product is NOT an essential feature of the mathematical definition of a vector space. A vector space can have many different inner products (or none).

In analogy with dot products, we call the square root of the inner product of a vector with itself $\langle v | v \rangle$ the **norm** or the **length** of the vector. Similarly, if the inner product of two vectors is zero $\langle v | w \rangle = 0$ we say that the vectors are **orthogonal** or **perpendicular** even when these statements have no obvious geometric meaning.

14.3 Visualizing the Dot Product in Higher Dimensions

The figure below shows a representation of the dot product in five dimensions, similar to the one given in Section 1.9. However, unlike that two-dimensional representation, we can not display the five (vector) components as orthogonal arrows. Instead, the sliders control the values of the (scalar) components, with the five components of $\vec{\boldsymbol{v}}$ shown on the left in brown, and the five components of $\vec{\boldsymbol{w}}$ shown on the right in blue. As in Figure 1.9.1, the histogram boxes provide a visual representation of the selected components, with corresponding products shown in green.

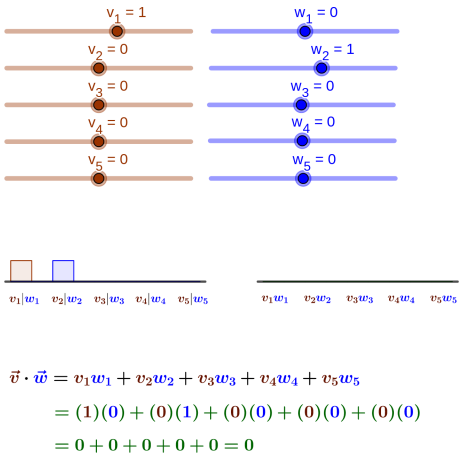


Figure 14.3.1 A representation of the dot product in five dimensions.

The same technique can be used to represent the dot product in any (relatively small) number of dimensions. This representation is based on the algebraic formula (1.8.5) for the dot product, and assumes that the vectors are expressed in terms of an orthonormal basis.

14.4 Visualizing the Product of Two Functions

The applet below shows the graph of the product fg (in green) of two functions f (in brown) and g (in blue). [1] This graph can be constructed by pointwise multiplication: At each point in the domain, read off the values of the two functions from their graphs, multiply these values together, and plot that value.

[1] The integral of the product is also shown; see Section 14.6.

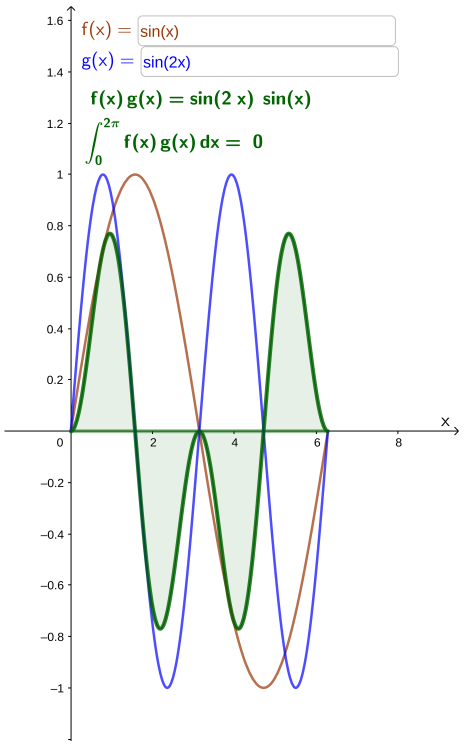


Figure 14.4.1 The product of two functions.

Activity 14.4.1 Multiplying Functions Together. Try it for yourself! Choose any two functions and graph them on the same axes. Looking only at these graphs, construct the graph of the product of the two functions. *After* completing this geometric construction, multiply the two functions together and graph the result. Did you draw the correct graph?

Hint. You can check your answer by entering the functions into the applet in Figure 14.4.1.

14.5 Inner Products of Harmonic Functions

What happens if you multiply two different trig functions, for example $\sin(2\theta)\sin(3\theta)$, as shown in Figure 14.5.1. As you might expect, there are two wave structures superposed. The overall structure (often called an envelope) of a large wave controlled by the difference of the two wavelengths and with smaller "wiggles" controlled by the sum of the two wavelengths.

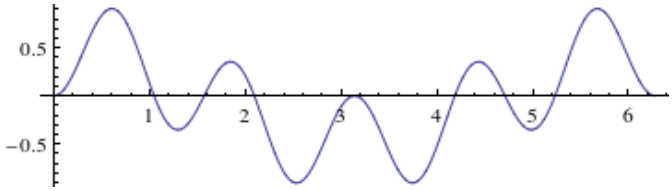


Figure 14.5.1 The graph of $y = \sin(2\theta)\sin(3\theta)$.

For Fourier series, what we will care about is the area under this graph. What is the integral of this combined function? Hard to tell, but there's about as much area above the axis as below, so zero would be plausible guess, which turns out to be correct. This central identity underlies all of Fourier theory.

It is in fact not that difficult to evaluate such integrals in closed form. Using technology or integral tables, we find the indefinite integral

$$\int \cos(m\theta)\cos(n\theta)\,d\theta = \frac{m\,\sin(m\theta)\cos(n\theta) - n\,\cos(m\theta)\sin(n\theta)}{m^2 - n^2} \tag{14.5.1}$$

for $m \neq n$. There are similar formulas for the various combinations of sines and cosines. You should notice that we will need to be careful when $m \neq n$.

For Fourier series, we care about the cases where m and n are both integers, and we want the definite integral over an entire period; with these assumptions, we find

$$\int_0^{2\pi} \sin(m\theta)\sin(n\theta)\,d\theta = \delta_{mn}, \tag{14.5.2}$$

$$\int_0^{2\pi} \sin(m\theta)\cos(n\theta)\,d\theta = 0, \tag{14.5.3}$$

$$\int_0^{2\pi} \cos(m\theta)\cos(n\theta)\,d\theta = \delta_{mn}. \tag{14.5.4}$$

where the Kronecker delta δ_{mn} is defined in Section 17.1.

To complete this list, we consider the case $m = 0$. (Since $\sin(0\,\theta)$ is the zero function, we do not need to include that case.) We get one last formula:

$$\int_0^{2\pi} \cos^2(0\,\theta)\,d\theta = 2\pi. \tag{14.5.5}$$

Activity 14.5.1 Integrals of products of harmonic functions. Use Euler's formula (2.6.1) to find the values of the definite integrals in this section by hand, by explicitly integrating exponential functions.

14.6 Inner Products of Functions

The applet below shows the product (see Section 14.4) of two trigonometric functions whose periods are related by a factor of 2. There is about as much area above the graph of this product as below, so it is plausible that the integral of this product should be 0, which turns out to be correct. This result holds for the product of *any* two sine or cosine functions whose periods are related by a rational number other than 1, so long as the integral is taken over (a multiple of) a full period of both functions.

In the applet shown, with the integral being taken from 0 to 2π, this condition is equivalent to requiring the coefficients of x to be distinct integers. (The integers can be the same if one function involves sine and the other cosine.)

You can verify this remarkable fact by inserting any two distinct integers into the functions in the applet, and/or changing one or both functions from cosine to sine. What happens if you use the same integer twice?

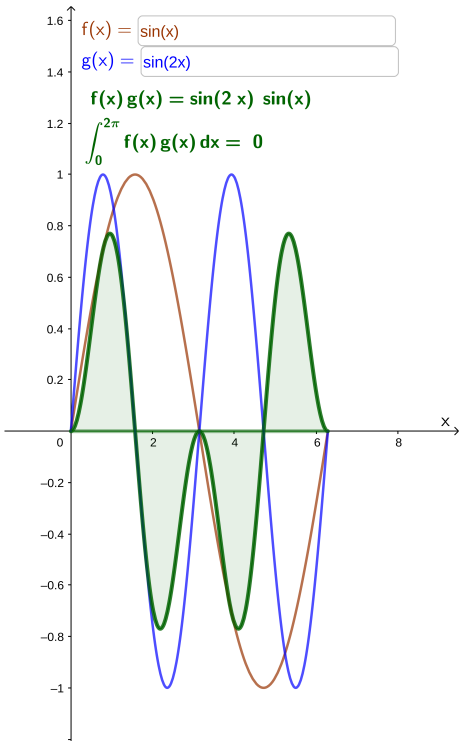


Figure 14.6.1 The product of two trigonometric functions.

You can check that these periodic functions satisfy the conditions to be interpreted as "vectors" in an abstract vector space (see Section 14.1), and the integral satisfies the conditions to be interpreted as a "dot" or inner product (see Section 14.2). The sines and cosines above are orthogonal! We can therefore use these functions as a natural basis for this vector space of periodic functions. We will discuss this example vector space further in a chapter on Fourier series, Chapter 20.

Definition 14.6.2 Inner Product for Fourier Series. More formally, there is an **inner product** (see Section 14.2) on (suitably smooth, periodic) functions given by

The "bra-ket" notation used here is often used in quantum mechanics and is further discussed in Section 14.2. In the context of real functions, such as those considered here, the complex conjugation doesn't do anything, but is included anyway to better match the notation used in more general contexts.

$$\langle f|g\rangle = \int_0^{2\pi} f^*(x)g(x)\,dx \tag{14.6.1}$$

under which the functions $\{1, \cos nx, \sin nx\}$ are **orthogonal**. However, they are not normalized, as you can verify using the applet above. ◊

Periodic functions with sines and cosines as the basis are not the only set of functions that are vector spaces. There are many others, typically associated with a particular differential equation with a particular boundary condition. Each such vector space has a natural inner-product defined on it, similar to (14.6.1) above. The study of these vector spaces as they arise in partial differential equations is called **Sturm-Liouville theory**.

14.7 Completeness

Given a vector and an orthonormal basis, it is easy to determine the components of the vector in the given basis. For example, if

$$\vec{\boldsymbol{F}} = F_x\,\hat{\boldsymbol{x}} + F_y\,\hat{\boldsymbol{y}} + F_z\,\hat{\boldsymbol{z}} \tag{14.7.1}$$

then dotting both sides of this equation with $\hat{\boldsymbol{x}}$ yields the x-component of the vector, namely F_x.

$$\begin{aligned}\hat{\boldsymbol{x}}\cdot\vec{\boldsymbol{F}} &= \hat{\boldsymbol{x}}\cdot(F_x\,\hat{\boldsymbol{x}} + F_y\,\hat{\boldsymbol{y}} + F_z\,\hat{\boldsymbol{z}}) \\ &= F_x\,\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{x}}^{1} + F_y\,\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{y}}^{0} + F_z\,\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{z}}^{0} \\ &= F_x\end{aligned} \tag{14.7.2}$$

where the orthonormality of the basis vectors has been used in the middle step.

Put differently,

$$\vec{\boldsymbol{F}} = (\vec{\boldsymbol{F}}\cdot\hat{\boldsymbol{x}})\,\hat{\boldsymbol{x}} + (\vec{\boldsymbol{F}}\cdot\hat{\boldsymbol{y}})\,\hat{\boldsymbol{y}} + (\vec{\boldsymbol{F}}\cdot\hat{\boldsymbol{z}})\,\hat{\boldsymbol{z}}. \tag{14.7.3}$$

All we need to make this idea work is an orthonormal basis. (If the basis is not normalized, the method still works, but we will need to account for the normalization of the basis vectors explicitly.)

In function spaces, for example for Fourier series in Section 14.6, the sum in the dot product above becomes an integral. The orthogonal basis elements are the trigonometric functions

$$\{1, \cos nx, \sin nx\} \tag{14.7.4}$$

with n a positive integer. There are an infinite number of basis vectors! But what vector space do they span?

Definition 14.7.1 Completeness. For a finite dimensional vector space, it is usually obvious how many vectors are required to make a basis, i.e. the minimum number of vectors you need to ensure that every vector can be built out of a linear combiniation of the basis. For example, for arrows in 3-dimensional space, we need three basis vectors. That's what the number 3 in "3-dimensional" means. The technical language for this concept is that this basis is **complete**. For an infinite dimensional vector space, such as periodic functions, the proof of what makes a basis complete is more difficult. Fortunately, mathematicians have all ready done the proofs in the applied cases that we care about, so it is only necessary to know the result. It turns out that the any periodic function that is reasonably well behaved (for instance, piecewise smooth) can be expanded uniquely in terms of the basis given in (14.7.4). This basis is complete on the vector space of (piecewise smooth) periodic functions with period 2π. ◊

14.8 Linear Operators: Definitions and Examples

Definition 14.8.1 Linear Operator. An operator $\mathcal{L}$ is **linear** if it satisfies two conditions when acting on any appropriate vector v and for any constants α:

$$\mathcal{L}(\alpha v) = \alpha\mathcal{L}v \tag{14.8.1}$$

$$\mathcal{L}(v_1 + v_2) = \mathcal{L}v_1 + \mathcal{L}v_2 \tag{14.8.2}$$

$\Diamond$

Derivatives Are Linear Operators. You have often used the fact that the derivative operator acting on functions is linear:

$$\frac{d}{dx}(\alpha f) = \alpha\left(\frac{d}{dx}f\right) \tag{14.8.3}$$

$$\frac{d}{dx}(f+g) = \left(\frac{d}{dx}f\right) + \left(\frac{d}{dx}g\right) \tag{14.8.4}$$

For example,

$$\frac{d}{dx}\left(3x^2 + \cos x\right) = 3\frac{d}{dx}x^2 + \frac{d}{dx}\cos x \tag{14.8.5}$$

To prove linearity, you would need to look at the details of the limit definition of the derivative. It's not hard, try it!

By a straightforward extension, the differential operator $\mathcal{L}$ defined by

$$\mathcal{L} \equiv a_n(x)\frac{d^n}{dx^n} + a_{n-1}(x)\frac{d^{n-1}}{dx^{n-1}} + \cdots + a_0(x) \tag{14.8.6}$$

is also *linear*. The important feature here is that all of the (nth order) derivatives are to the first power and not inside of any other special functions. (Do not be confused by the notation for nth order derivatives, which looks like the notation for the nth power.) Many differential operators in physics ARE linear, so this should look very comfortable and familiar. As counterexamples, the following strange-looking differential operators are NOT linear:

$$\left(\frac{d}{dx}f\right)^2, \tag{14.8.7}$$

$$\sin\left(\frac{d}{dx}f\right). \tag{14.8.8}$$

In particular, you may have seen the equation for the motion of a pendulum:

$$\frac{d^2\theta}{dt^2} + \frac{g}{L}\sin\theta = 0 \tag{14.8.9}$$

The term $\sin\theta$ makes this equation non-linear. When you make the small angle approximation (the first term in a power series expansion) $\sin\theta \approx \theta$, the equation becomes linear, and therefore simple to solve. (See Section 15.6 for the method of solving this equation.) But the solution is only approximately true and the approximation is best when the angle θ is small.

Other Examples of Linear Operators. You use the fact that **matrix multiplication** (acting on vectors that are columns and multiplication by scalars α) is a linear operator when you do the following common matrix manipulations.

$$\begin{pmatrix}2 & 3\\ 4 & 5\end{pmatrix}\left(\alpha\begin{pmatrix}6\\7\end{pmatrix}\right) = \alpha\left(\begin{pmatrix}2 & 3\\ 4 & 5\end{pmatrix}\begin{pmatrix}6\\7\end{pmatrix}\right) \tag{14.8.10}$$

$$\begin{pmatrix}2 & 3\\ 4 & 5\end{pmatrix}\left(\begin{pmatrix}6\\7\end{pmatrix} + \begin{pmatrix}8\\9\end{pmatrix}\right) = \left(\begin{pmatrix}2 & 3\\ 4 & 5\end{pmatrix}\begin{pmatrix}6\\7\end{pmatrix}\right) + \left(\begin{pmatrix}2 & 3\\ 4 & 5\end{pmatrix}\begin{pmatrix}8\\9\end{pmatrix}\right) \tag{14.8.11}$$

You also use the fact that **Hermitian operators** in quantum mechanics, for example, the Hamiltonian, are linear when you do the following bra/ket manipulations.

The most common representations for the Hamiltonian are as linear differential operators or as matrix operators, so this example is really just an abstraction of the previous two examples.

$$H\left(\alpha|\psi\rangle\right) = \alpha\left(H|\psi\rangle\right) \tag{14.8.12}$$
$$H\left(\alpha|\psi_1\rangle + \alpha|\psi_2\rangle\right) = \left(H|\psi_1\rangle\right) + \left(H|\psi_2\rangle\right) \tag{14.8.13}$$

14.9 Linear Operators (Advanced)

Origin of the Word "Linear" in Linear Operator. The word linear comes from linear equations, i.e. equations for straight lines. The equation for a line through the origin $y = mx$ comes from the operator $f(x) = mx$ acting on vectors which are real numbers x and constants that are real numbers α. The first property:

$$f(\alpha x) = m(\alpha x) = \alpha(mx) = \alpha f(x) \tag{14.9.1}$$

is just commutativity of the real numbers. The second property:

$$f(x_1 + x_2) = m(x_1 + x_2) = m(x_1) + m(x_2) = f(x_1) + f(x_2) \tag{14.9.2}$$

is just distributivity of multiplication over addition. These are properties of real numbers that you've used since grade school, even if you didn't know to call the properties by these fancy names! Note that the equation for a line NOT through the origin $y = mx + b$, leading to the operator $g(x) = mx + b$, is NOT linear.

$$g(x_1+x_2) = m(x_1+x_2)+b \neq (mx_1+b)+(mx_2+b) = g(x_1)+g(x_2). \tag{14.9.3}$$

Inhomogeneous Linear Differential Equations. It will be helpful to remember the example of linear equations with zero and non-zero y-intercept when you are learning the difference between homogeneous and inhomogeneous linear differential equations in Section 15.1.

As with the example above for straight lines through the origin and not through the origin, if you take a homogeneous linear differential operator $\mathcal{L}$ as in example 1 above and add to it an inhomogeneous term $b(x)$, the resulting operator which takes y to $\mathcal{L}y - b(x)$ is NOT linear. If y_p and y_q are both solutions of

$$\mathcal{L}y = b(x), \tag{14.9.4}$$

then

$$\mathcal{L}\left(y_p + y_q\right) = 2b(x) \neq b(x). \tag{14.9.5}$$

You can NOT add two solutions of an inhomogeneous differential equation and get another solution. However, you CAN add ANY solution of the homogeneous equation to a solution of the inhomogeneous equation to get another solution of the inhomogeneous equation.

Chapter 15

Ordinary Differential Equations

15.1 Definitions

In this section, we define several different types of differential equations and discuss their properties.

Definition 15.1.1 Differential Equations. A **differential equation** is an equation involving an unknown function and its derivatives. A differential equation is an **ordinary differential equation (ODE)** if the unknown function depends on only one independent variable. If it depends on more than one variable, the equation is a **partial differential equation (PDE)**. The **order** of a differential equation is the order (number of derivatives taken) of the highest derivative appearing in the equation. The **degree** of a differential equation that can be written as a polynomial in the unknown function and its derivatives is the power to which the highest order derivative is raised. ◊

A simple example of a second-order ordinary differential equation is

$$\frac{d^2y}{dx^2} = a \tag{15.1.1}$$

where a is a constant. This simple example can be solved by integrating both sides twice.

Definition 15.1.2 Linearity and Homogeneity. An n^{th} order differential equation is **linear** if it has the form

$$a_n(x)y^{(n)}(x) + a_{n-1}(x)y^{(n-1)}(x) + \cdots + a_0(x)y(x) = b(x). \tag{15.1.2}$$

A linear equation is **homogeneous** if $b(x) = 0$ and **inhomogeneous** if $b(x) \neq 0$. ◊

The example above is inhomogeneous unless $a = 0$, in which case it is homogeneous.

Notation 15.1.1 Linear Differential Operators. To simplify differential equations such as (15.1.2), it is common to pull out all the derivative operators with their coefficients into a single **differential operator** acting on the unknown function y. Thus, the big messy operator gets replaced by the single

caligraphic letter $\mathcal{L}$, where

$$\mathcal{L} \equiv a_n(x)\frac{d^n}{dx^n} + a_{n-1}(x)\frac{d^{n-1}}{dx^{n-1}} + \cdots + a_0(x) \tag{15.1.3}$$

so that (15.1.2) becomes

$$\mathcal{L}y(x) = b(x). \tag{15.1.4}$$

By convention, the differential operator $\mathcal{L}$ is always written to the left of the function that it acts on.

In the example above, $\mathcal{L} = \frac{d^2}{dx^2}$.

Definition 15.1.3 Solution (of a differential equation). A **solution** of a differential equation in the unknown function y and the independent variable x on the interval I is a function $y(x)$ that satisfies the differential equation identically for all x in I. A **particular** solution of a differential equation is any one solution. The **general solution** is the set of all solutions, typically expressed in terms of free parameters. ♢

The general solution of the example differential equation is $y = \frac{a}{2}x^2 + bx + c$, where b and c are free parameters, that is, constants that can take on any value.

Definition 15.1.4 Initial and Boundary Value Problems. An **initial value problem** is a differential equation together with conditions (known as initial conditions) on the unknown function and its derivatives all at the same value of the independent variable. A **boundary value problem** is a differential equation together with conditions (known as boundary conditions) on the unknown function and its derivatives at more than one value of the independent variable. ♢

The constants b and c could be determined by specifying either the initial values $y(0)$ and $y'(0)$ or the boundary values $y(x_1)$ and $y(x_2)$.

15.2 First-Order ODEs: Forms and Theorems

First-order ODEs (Section 15.1) are among the simplest. For fairly general smoothness conditions, a solution is not only guaranteed to exist, but is also guaranteed to be unique. The technical theorem is stated below, but you may want to regard this as a *Don't Worry about It* theorem. It tells you that you can just go ahead and try to solve it by one of the analytical methods listed in the next couple of sections. If you find a solution, then it exists and is unique. Usually, any limitations on WHERE it exists will be obvious from the physical situation.

The theorem may become more important to you if you are trying to find a numerical solution to the ODE. Numerical methods can inadvertently jump over a place where the solution does not exist and lead you to believe, incorrectly, that two solutions that are perfectly valid in adjacent regions are also valid across the boundary between them. This theorem will help you identify the boundary.

There are a number of different methods for solving these equations. Which one you may want to use depends on the form of the equation. Listed here are some common forms of first-order ODEs:

Definition 15.2.1 Forms of First-Order ODEs.

Standard Form: You can ALWAYS write a first-order ODE in standard

form:

$$\frac{dy}{dx} = f(x, y). \tag{15.2.1}$$

In this form, you are isolating the derivative term on one side of the equation, which may involve some really messy inverse functions on the other side of the equation. Because it can be messy, this form is used primarily in the statement of theorems about existence and uniqueness of solutions.

Separable Form: If you can write

$$f(x, y) = h(x)g(y), \tag{15.2.2}$$

then Eqn(15.2.1) is called separable. It is NOT always possible to write the equation in this form, but when you can, the solution is straightforward. See Section 15.3 for a discussion of the solution method.

Differential Form: If you write the standard form equation as

$$f(x, y) = -\frac{M(x, y)}{N(x, y)}, \tag{15.2.3}$$

then with some straightforward algebraic rearrangement, Eqn(15.2.1) becomes the differential form

$$M(x, y)\, dx + N(x, y)\, dy = 0 \tag{15.2.4}$$

There are many ways to divide $f(x, y)$ into $M(x, y)$ and $N(x, y)$. Choose a way that is helpful for the problem at hand. In particular, you can ALWAYS choose $M(x, y)$ and $N(x, y)$ so that (15.2.4) is an exact differential and the equation can be solved by simple integration. See Section 15.4 for a discussion of this solution method. ◊

Theorem 15.2.2 First-Order ODEs: Uniqueness Theorem. *If f and $\frac{\partial f}{\partial y}$ are continuous in a rectangle $|x - x_0| \le a$, $|y - y_0| \le b$, then there exists an interval about x_0 in which the initial value problem $y' = f(x, y)$, $y(x_0) = y_0$ has a unique solution.*

To Remember. Under physically reasonable circumstances, the solution of a first-order ODE exists and is unique. If you can find a solution by any convenient method, you can be confident that it is THE solution.

15.3 Separable ODEs

Separable ODEs are first order ODEs with the special form:

$$\frac{dy}{dx} = h(x)g(y). \tag{15.3.1}$$

where $h(x)$ and $g(y)$ are arbitrary functions, i.e. the x and y dependencies are separated into the product of two functions. A solution will exist wherever these functions are sufficiently smooth and y has no values for which $g(y)$ is zero.

Method. First, write (15.3.1) as a differentials equation by multiplying through by dx. Then divide by $g(y)$ so that all the y-dependence is on one side of the equation and all the x-dependence is on the other side of the equation. Finally, integrate both sides of the equation.

$$dy = h(x)g(y)\, dx, \tag{15.3.2}$$

$$\frac{1}{g(y)}\,dy = h(x)\,dx, \tag{15.3.3}$$

$$\int \frac{1}{g(y)}\,dy = \int h(x)\,dx. \tag{15.3.4}$$

You may or may not be able to solve the resulting implicit equation for the dependent variable, in this case y.

If you do the integral as an indefinite integral, don't forget to add an arbitrary constant. (Adding the constant to one side of the equation is sufficient.) If you know an initial or boundary condition, the integrals become definite integrals and you can use this information to specify the value of the unknown constant.

Activity 15.3.1 Solve the differential equation

$$\frac{dy}{dx} = y\,(3x-2)\,. \tag{15.3.5}$$

Answer.

$$y = e^{\left(\frac{3x^2}{2}-2x+C\right)} \tag{15.3.6}$$

Solution. Following the method above, we have

$$dy = (3x-2)\;dx, \tag{15.3.7}$$

$$\frac{1}{y}\,dy = (3x-2)\;dx, \tag{15.3.8}$$

$$\int \frac{1}{y}\,dy = \int (3x-2)\;dx. \tag{15.3.9}$$

$$\ln y = \frac{3x^2}{2} - 2x + C. \tag{15.3.10}$$

If we are given an initial condition such as $y(0) = 7$, then we can use this to find the value $C = \ln 7$. The final answer is

$$\ln y = \frac{3x^2}{2} - 2x + \ln 7, \tag{15.3.11}$$

$$y = e^{\left(\frac{3x^2}{2}-2x+\ln 7\right)}, \tag{15.3.12}$$

$$= 7e^{\left(\frac{3x^2}{2}-2x\right)}. \tag{15.3.13}$$

15.4 Exact ODEs

COMING SOON! For now, see Boas 6.8 and 8.4

Note: Any first order linear ODE can be solved on some interval. You can always multiply the differential form of the differential equation by an appropriate function of the independent and dependent variables (called an integrating factor) so that the equation becomes exact. Then you can solve the differentials equation using methods for exact equations. Boas 8.3 has a nice description that not only shows you how to find the integrating factor, but also shows you how to find the solution of the differential equation in terms of that integrating factor.

15.5 Theorems about Linear ODEs

In this section, we will give, without proof, several important theorems about linear differential equations. But before we get to the theorems, you will need to understand what is meant by the word *linear*, see Section 14.8. so that you can understand the content of these theorems. Before you read this section, you should also make sure you know the definitions and notation in Section 15.1.

The first two theorems tell us the general form for solutions for homogeneous and inhomogeneous linear differential equations and describe the free parameters that exist in each solution. The third theorem describes what kind of initial conditions are necessary to remove this freedom and specify a unique solution.

Theorem 15.5.1 Linear Homogeneous ODEs: Form of General Solution. *An n^{th} order linear* homogeneous *differential equation $\mathcal{L}(y) = 0$ always has n linearly independent solutions, $y_1, \ldots, y_n$. The general solution y_h is*

$$y_h = C_1 y_1 + C_2 y_2 + \cdots + C_n y_n \tag{15.5.1}$$

where $C_1, C_2, \ldots, C_n$ are arbitrary *constants. Technically, the space of all solutions forms an n-dimensional vector space, see Section 14.1.*

Theorem 15.5.2 Linear Inhomogeneous ODEs: Form of General Solution. *The* general *solution of the n^{th} order linear* inhomogeneous *differential equation $\mathcal{L}(y) = b(x)$ is*

$$y = y_h + y_p \tag{15.5.2}$$

where y_h is the general solution of the homogeneous equation $\mathcal{L}(y) = 0$ and y_p is any one *particular solution of the inhomogeneous equation. Recall that the general solution of the homogeneous equation (above) has n independent parameters.*

Theorem 15.5.3 Linear ODEs: What Initial Conditions Make the Solution Unique. *Consider the n^{th} order, linear, ordinary differential equation:*

$$1y^{(n)} + a_{n-1}(x)y^{(n-1)} + \cdots + a_0(x)y = b(x) \tag{15.5.3}$$

Note the coefficient 1 in front of the $y^{(n)}$ term.

together with the initial conditions:

$$y(x_0) = c_0 \tag{15.5.4}$$
$$y'(x_0) = c_1 \tag{15.5.5}$$
$$\vdots$$
$$y^{(n)}(x_0) = c_n \tag{15.5.6}$$

If $b(x)$ and $a_j(x)$ are continuous $\forall j$ on some interval I containing x_0, then the initial value problem has a unique solution throughout I.

15.6 Constant Coefficients, Homogeneous, Linear ODEs

Form of the equation. Consider an nth order linear ODE of the form

$$a_n \frac{d^n y}{dx^n} + a_{n-1} \frac{d^{n-1} y}{dx^{n-1}} + \ldots + a_0 y = 0 \tag{15.6.1}$$

where the coefficients a_i are *constant*. This very special case of the general nth order linear ODE, for which all of the a_i's are constant, comes up in physics incredibly often. Especially important is the case of small, (damped, for $b \neq 0$) oscillations, such as for a pendulum, which are described by a second order linear ODE ($n = 2$), using the independent variable t:

$$\frac{d^2\theta}{dt^2} + 2b\,\omega_0 \frac{d\theta}{dt} + \omega_0^2\theta = 0 \tag{15.6.2}$$

It will be important that you recognize this equation whenever it comes up, regardless of the algebraic letters that are used. Look for *second order*, *linear*, *homogeneous*, and CONSTANT coefficients. Reread this section 15.1of the book if you need to review the meaning of any of these words.

Method. Definition 15.6.1 ***Ansatz.*** Often, when we are solving differential equations, we make an ***ansatz***, i.e. an initial guess for the basic form of the solution with some unknown parameters or functions. We then plug the guess into the differential equation to get a simpler equation for the unknown parameters. ◊

The differential equation eqn. (15.6.1) can be solved by making the *ansatz*

$$y = e^{kx} \tag{15.6.3}$$

where k is an unknown constant. We will find the value of the unknown k by substituting this expression back into the original equation. This *ansatz* is a reasonable guess because the derivative of e^{kx} is just a multiple of itself and higher order derivatives

$$\frac{d^m e^{kx}}{dx^m} = k^m e^{kx} \tag{15.6.4}$$

are also multiples of the original function. Each term of equation (15.6.1) after substitution will have a factor of e^{kx}, i.e. we obtain

$$\left(k^n + a_{n-1}k^{n-1} + ...a_0\right) e^{kx} = 0 \tag{15.6.5}$$

Definition 15.6.2 Characteristic Polynomial Equation. After we factor out e^{kx}, the differential equation has been reduced to the **characteristic polynomial equation**

$$a_n k^n + a_{n-1}k^{n-1} + ...a_0 = 0 \tag{15.6.6}$$

for the unknown parameter k. ◊

The **characteristic equation** is a huge simplification! The ODE (15.6.1) has become a polynomial equation (15.6.6), which is much easier to solve. Notice that the order of the original ODE, namely n, is also the order of the characteristic polynomial. Over the complex numbers, nth order polynomials have exactly n roots which may be degenerate (i.e there may be repeated roots, see Section A.2). If there is no degeneracy, then we obtain n linearly-independent solutions of the nth-order differential equation by plugging in each of the different values of k into the *ansatz*. If there is degeneracy, we need to do something a little trickier to get n linearly independent solutions. See Section 15.6.2.

There is a theorem, which we quote without proof, that says that the trick below always works and we can obtain n solutions in both the non-degenerate and degenerate cases.

Theorem 15.6.3 Solutions of ODEs with Constant Coefficients. *A homogeneous nth-order ordinary differential equation with constant coefficients admits exactly n linearly-independent solutions. Therefore, the general solution will have n unknown parameters that can be specified with initial conditions or boundary conditions.*

Activity 15.6.1 Generic Example. Find the general solution of:

$$\frac{d^2y}{dx^2} + \frac{dy}{dx} - 6y = 0. \tag{15.6.7}$$

Answer.

$$y = C_1e^{-3x} + C_2e^{2x} \tag{15.6.8}$$

Solution. Substituting (15.6.3) into (15.6.7) leads to

$$0 = k^2 + k - 6 = (k+3)(k-2) \tag{15.6.9}$$

so that $k = -3$ or $k = 2$. You should check that both e^{-3x} and e^{2x} do indeed satisfy (15.6.7); the general solution of this *homogeneous* ODE is given by

$$y = C_1e^{-3x} + C_2e^{2x} \tag{15.6.10}$$

for arbitrary constants C_i.

Activity 15.6.2 Special Case: Repeated Roots. Find the general solution of:

$$\frac{d^2y}{dx^2} - 2\frac{dy}{dx} + y = 0? \tag{15.6.11}$$

Answer.

$$y = C_1e^{x} + C_2xe^{x} \tag{15.6.12}$$

Solution. In this case, the characteristic polynomial is

$$0 = k^2 - 2k + 1 = (k-1)^2 \tag{15.6.13}$$

and indeed e^x does satisfy (15.6.11). But wait a minute—that's only one solution! This is a second order equation, so the theorem above guarantees a second solution. How do we find it?

There's a trick in the case of repeated roots (degeneracy), which we will state without proof. The extra solutions are of the form $x^me^{\alpha x}$. In this case, the second solution is $x\,e^{\alpha x}$; in general, the other linearly independent solutions include terms with $m = 0, 1, ..., r-1$ for a root of multiplicity r.

For example (15.6.11), the general solution is:

$$y = C_1e^{x} + C_2xe^{x} \tag{15.6.14}$$

Activity 15.6.3 Special Case: Complex Roots. Find the general solution of:

$$\frac{d^2y}{dx^2} + 4y = 0 \tag{15.6.15}$$

Answer. We can write the general solution of (15.6.15) in two ways:

$$y = C_1e^{2ix} + C_2e^{-2ix} \tag{15.6.16}$$

$$= D_1\cos 2x + D_2\sin 2x \tag{15.6.17}$$

Solution. Even if the coefficients of the ODE are real, some of the roots of the characteristic polynomial could be complex. In this case, the independent

solutions are $y = e^{\pm 2ix}$. Since such complex solutions always come in pairs if the coefficients are real (Why?), we can use Euler's formula to replace the complex exponentials by trig functions, which in this case are

$$\cos(2x) = \frac{1}{2}(e^{2ix} + e^{-2ix}), \tag{15.6.18}$$

$$\sin(2x) = \frac{1}{2i}(e^{2ix} - e^{-2ix}). \tag{15.6.19}$$

We can write the general solution of (15.6.15) in two ways:

$$\begin{aligned} y &= C_1 e^{2ix} + C_2 e^{-2ix} \\ &= C_1 (\cos 2x + i \sin 2x) + C_2 (\cos 2x - i \sin 2x) \\ &= D_1 \cos 2x + D_2 \sin 2x \end{aligned} \tag{15.6.20}$$

There is, of course, a simple relationship between the pairs of coefficients C_1, C_2 and D_1, D_2, but since these coefficients are unknown until we specify the boundary conditions or initial conditions, we rarely need to solve for this relationship. Once you understand the relationship between these two solutions, you can of course always just write down the second solution instead of the first, without going through the algebraic steps in (15.6.20).

In the language of vector spaces (see Chapter 14), the algebraic steps in (15.6.20) are just a change of basis in the two-dimensional vector space of solutions.

15.7 Linear Independence

Motivation and Analogy. We know from the theorem quoted in Theorem 15.5.2 on nth order linear homogeneous differential equations $\mathcal{L}y = 0$ that the general solution is a linear combination of n linearly independent solutions

$$y = C_1 y_1 + C_2 y_2 + \cdots + C_n y_n \tag{15.7.1}$$

What does the word *linearly independent* mean and how do we find out if a set of particular solutions *is* linearly independent?

Let's examine a close geometric analogy. Consider the set of three vectors in the plane

$$\{\vec{v}_1 = \hat{x}, \vec{v}_2 = \hat{y}, \vec{v}_3 = 3\hat{x} - 2\hat{y}\}. \tag{15.7.2}$$

Notice that the third vector is a linear combination of the first two:

$$\vec{v}_3 = 3\vec{v}_1 - 2\vec{v}_2 \tag{15.7.3}$$

or

$$3\vec{v}_1 - 2\vec{v}_2 - \vec{v}_3 = 0. \tag{15.7.4}$$

We say that these three vectors are *linearly dependent* (alternatively, *NOT linearly independent*). Geometrically, this is equivalent to the statement that these three vectors lie in a two-dimensional plane.

Why is linear independence important? If we wanted to expand another vector $\vec{v}_4$, it is sufficient to expand it in terms of the linearly independent vectors $\vec{v}_1$ and $\vec{v}_2$:

$$\vec{v}_4 = D_1\vec{v}_1 + D_2\vec{v}_2 \tag{15.7.5}$$

and the coefficients D_1 and D_2 are unique. We say that $\vec{v}_1$ and $\vec{v}_2$ form a basis for the two-dimensional vector space. We do not need to include the vector $\vec{v}_3$ in the expansion,

$$\vec{v}_4 = D_1\vec{v}_1 + D_2\vec{v}_2 + D_3\vec{v}_3 \tag{15.7.6}$$

but if we did include it the coefficients D_1, D_2, and D_3 would not be uniquely specified. Many combinations of Ds would work.

We will now extend this definition of linear independence of vectors that are arrows in space to linear independence of functions that are solutions of a linear ODE. There is deep mathematics underlying the analogy. The solutions of a linear ODE form a vector space (see Section 14.1).

Definition 15.7.1 Linear Independence of Functions. A set of n functions $y_1, \ldots, y_n$ on an interval I are *linearly dependent* if there exist constants $C_1, C_2, \ldots, C_n$, not all zero, such that

$$C_1 y_1 + C_2 y_2 + \cdots + C_n y_n = 0 \tag{15.7.7}$$

Otherwise the functions are *linearly independent.* ◊

Testing for Linear Independence: Wronskians. It is cumbersome to use the definition above to find out if a set of functions is linearly independent. If the set of functions are all solutions of the same linear ODE, then there is a much quicker method, using a mathematical object called a Wronskian. *Definition:* If a set of n functions $y_1, \ldots, y_n$ on an interval I each have $n-1$ derivatives, then the determinant $W(y_1, \ldots, y_n)$, defined below, is called the *Wronskian* of the set of functions.

$$W(y_1, \ldots, y_n) \doteq \begin{vmatrix} y_1 & y_2 & \cdots & y_n \\ y_1' & y_2' & \cdots & y_n' \\ \vdots & \vdots & \vdots & \vdots \\ y_1^{(n-1)} & y_2^{(n-1)} & \cdots & y_n^{(n-1)} \end{vmatrix} \tag{15.7.8}$$

Theorem: If $y_1, \ldots, y_n$ are solutions of $\mathcal{L}(y) = 0$ on I, then they are linearly independent $\iff$ $W(y_1, \ldots, y_n)$ is *not* identically zero on I.

Note: This theorem is only valid if the functions $y_1, \ldots, y_n$ are all solutions of the *same* n^{th} order linear ODE.

A Note on Orthonormality. Just as with vectors that are arrows in space, it is often convenient, but not necessary to choose the linearly independent basis functions to be orthonormal, i.e. orthogonal and normalized. In the motivation section above, I chose to focus on $\vec{v}_1 = \hat{x}$ and $\vec{v}_2 = \hat{y}$ as the basis because that is the conventional orthonormal basis, but everything I said would have worked perfectly well if I had chosen $\vec{v}_1 = \hat{x}$ and $\vec{v}_3 = 3\hat{x} - 2\hat{y}$ as the basis instead. It just would have been a little harder for you to follow the algebra. In the same way, it will often simplify algebra for us if we choose the linearly independent basis functions to be orthonormal, but we'll need to generalize the ideal of the dot product to these functions. See section 14.5.

15.8 Constant Coefficients, Inhomogeneous

Form of the equation. An nth order linear differential equation with constant coefficients is *inhomogeneous* if it has a nonzero "source" or "forcing function," i.e. if it has a term that does NOT involve the unknown function. We will call this source $b(x)$. The form of these equations is:

$$a_n \frac{d^n y}{dx^n} + a_{n-1} \frac{d^{n-1} y}{dx^{n-1}} + \ldots + a_0 y = b(x)$$
$$\mathcal{L}y = b(x) \tag{15.8.1}$$

In the second form for these equations, we have rewritten all the messy derivative information as a linear differential operator $\mathcal{L}$ so that it is easier to see the important steps of the algebra below.

Strategy. The following theorem explains how you will know when you have the most general solution of these equations. The proof is simple and illustrative, it's worth reading.

Theorem 15.8.1 *An inhomogeneous nth-order ordinary differential equation with constant coefficients admits exactly n linearly-independent solutions. The general solution of the inhomogeneous equation is the sum of the general solution of the homogeneous equation y_h PLUS any one solution to the inhomogeneous equation, called a particular solution y_p.*

Proof. The general solution of the homogeneous equation satisfies $\mathcal{L}y_h = 0$ and the particular solution satisfies $\mathcal{L}y_p = b(x)$. Since the differential operator $\mathcal{L}$ is linear (see Section 14.8), it is straightforward to see that:

$$\begin{aligned} \mathcal{L}(y_h + y_p) &= \mathcal{L}y_h + \mathcal{L}y_p \\ &= 0 + b(x) \\ &= b(x) \end{aligned} \tag{15.8.2}$$

■

This theorem is telling us first to solve the homogeneous equation, which we know has n linearly independent solutions. The general solution will have n undetermined coefficients. Then we find one particular solution and add this and we're done.

Method/Simple Examples. So how do we find a particular solution to an inhomogenous ODE with constant coefficients? The general case is difficult and beyond the scope of this book. But it is easy to find particular solutions for the special cases that come up most often in physics. We will illustrate the method with examples.

Consider the ODE

$$\frac{d^2y}{dx^2} + \frac{dy}{dx} - 6y = e^{5x}. \tag{15.8.3}$$

Since derivatives of exponential functions are proportional to themselves, we choose an *ansatz* of the form

$$y_p = Ce^{5x}. \tag{15.8.4}$$

Notice that in this ansatz we are solving for the constant coefficient C, not the exponent as in section 15.6. The exponent is determined by the form of the inhomogeneous term.

Substituting (15.8.4) into (15.8.3), we obtain

$$(25C + 5C - 6C)\, e^{5x} = e^{5x} \tag{15.8.5}$$

which we can solve for C, yielding $C = 1/24$. Putting our particular solution (15.8.4) together with the general homogenous solution derived in Section 15.6, the general solution of (15.8.3) is

$$y = C_1e^{-3x} + C_2e^{2x} + \frac{1}{24}e^{5x} \tag{15.8.6}$$

Source terms that are trigonometric functions are similar, again recalling Euler's formula. Consider the ODE

$$\frac{d^2y}{dx^2} + 4y = \sin(3x). \tag{15.8.7}$$

The trick here is to recognize that $\sin(3x)$ involves both of $e^{\pm 3ix}$, so we had better incorporate both into our *ansatz*. However, we can do so by using trigonometric functions, rather than exponentials. Thus, we try a particular solution of the form

$$y_p = A\sin(3x) + B\cos(3x) \tag{15.8.8}$$

which results in

$$\begin{aligned} -9A\sin(3x) - 9B\cos(3x) + 4A\sin(3x) + 4B\cos(3x) &\qquad (15.8.9)\\ = \sin(3x). &\qquad (15.8.10) \end{aligned}$$

Collecting terms, and setting the coefficients of the linearly independent functions $\sin(3x)$ and $\cos(3x)$ separately to zero results in

$$\begin{aligned} -9A + 4A &= 1 \qquad (15.8.11)\\ -9B + 4B &= 0 \qquad (15.8.12) \end{aligned}$$

so that $A = -1/5$, $B = 0$ and our general solution is

$$y = C_1\cos(2x) + C_2\sin(2x) - \frac{1}{5}\sin(3x). \tag{15.8.13}$$

Typically, the particular solution will involve both sines and cosines. (Why doesn't that happen here?)

More General Cases. The method above will work for any single inhomogeneous term of the form $x^m e^{\alpha x}\cos\beta x$ or $x^m e^{\alpha x}\sin\beta x$, where m is a non-negative integer and α and β are real numbers, including possibly zero, with one *caveat*: since, in the differential equation, you will be taking derivatives of the proposed solution in the *ansatz*, the proposed solution should also contain terms of the same form as the derivatives, each with its own unknown constant. For example, if the inhomogeneous term is $x^2\cos 3x$, the proposed solution should be

$$\begin{aligned} &Ax^2\cos 3x + Bx\cos 3x + C\cos 3x\\ &\quad + Dx^2\sin 3x + Ex\sin 3x + F\sin 3x \end{aligned} \tag{15.8.14}$$

and you will need to solve for all of the constants $\{A, B, C, D, E, F\}$. (Keep differentiating until you don't get any terms with a new form.)

It is also possible to solve equations with more complicated inhomogeneous terms as long as the inhomogeneous term can be written as a linear combination of terms of the types above $b(x) = b_1(x) + b_2(x) + \ldots$. We just solve an inhomogeneous equation for each of the terms b_i separately and add the solutions $y_p = y_{p_1} + y_{p_2} + \ldots$. Notice how the linearity of the differential operator $\mathcal{L}$ guarantees that this method works in the following simple proof: Suppose $\mathcal{L}y_{p_i} = b_i$ for several values of the index i. Then:

$$\begin{aligned} \mathcal{L} &= \mathcal{L}(y_{p_1} + y_{p_2} + \ldots)\\ &= \mathcal{L}y_{p_1} + \mathcal{L}y_{p_2} + \ldots\\ &= b_1(x) + b_2(x) = \ldots\\ &= b(x) \end{aligned} \tag{15.8.15}$$

Relationship to Fourier Series and Power Series. If the inhomogeneous term is a periodic function, then we can expand it in a Fourier series (see Chapter 20). Once you learn to do Fourier Series, the method you have just learned becomes much more general, it applies to any periodic "source" or

"forcing function". Similarly, if the inhomogeneous term can be expanded in a power series (see Chapter 13), then this method will also work. So, we see that the method is actually quite general. Of course, if you only use a few terms of the Fourier or power series, then you will only get an approximate solution of the differential equation.

Chapter 16

Power Series Solutions of ODEs

16.1 Power Series Solutions: Method/Example

The power series method is one of the most powerful analytic methods that physicists have for solving linear differential equations. The idea is very simple, make an *ansatz* that a power series solution exists, but the coefficients in the power series are unknown. Plug this *ansatz* into the differential equation and use an iterative strategy to solve for the unknown coefficients. The method is easiest to see using a simple example:

Activity 16.1.1 A simple example of power series solutions of linear ODEs. Find a power series solution of

$$y' = Ay \tag{16.1.1}$$

for A a constant, expanded around the point $z = 1$.

Solution. *Ansatz*: Assume the solution *IS* a power series of the form:

$$y = \sum_{n=0}^{\infty} c_n (z-1)^n \tag{16.1.2}$$

Make sure that the powers that appear in the sum are powers of $z - z_0$, where z_0 is the point you are expanding around. Also, make sure that you use the correct name of the independent variable (in this case, the y' notation makes the independent variable unclear, so I have arbitrarily chosen z). And choose the correct name for the dependent variable (in this case, y).

Differentiating this expression, we obtain:

$$y' = \sum_{n=0}^{\infty} c_n \, n \, (z-1)^{n-1} \tag{16.1.3}$$

Now, rewrite Equation (16.1.1) so that all the terms are on the same side of the equation, then insert Equation (16.1.2) and Equation (16.1.3) to obtain:

$$0 = \sum_{n=0}^{\infty} c_n \, n \, (z-1)^{n-1} - A \sum_{n=0}^{\infty} c_n \, (z-1)^n \tag{16.1.4}$$

Now the strategy is to manipulate the indices n in the sums (in this case, just the first sum) so that each sum contains the same power of $z - z_0$ so that the sums can be combined into a single sum. Notice that each sum has

an index that is *summed over* so that the index does not appear in the final expression once the sum has been completed. This index is analogous to the variable of integration in a definite integral. Such an index is called a "dummy index" and you are free to rename it any way you want. On the first sum in Equation (16.1.4), rename $m = n - 1 \to n = m + 1$. Don't forget to change *every* n to an equivalent expression with ms, including the lower index in the sum.

$$0 = \sum_{m=-1}^{\infty} c_{m+1}\,(m+1)\,(z-1)^m - A\sum_{n=0}^{\infty} c_n\,(z-1)^n \tag{16.1.5}$$

Finally, relabel the dummy variable on the first sum, again: let $n = m$, so that the sums can be combined. Be careful, the limits of the sums are *not* the same, so you must separate out any extra terms that are in one sum and not the other.

$$0 = \sum_{n=-1}^{\infty} c_{n+1}\,(n+1)\,(z-1)^n - A\sum_{n=0}^{\infty} c_n\,(z-1)^n \tag{16.1.6}$$

$$= \sum_{n=-1}^{n=-1} c_{n+1}\,(n+1)\,(z-1)^n \tag{16.1.7}$$

$$+ \sum_{n=0}^{\infty} [c_{n+1}\,(n+1) - A\,c_n]\,(z-1)^n \tag{16.1.8}$$

The first term is identically zero when you plug in $n = -1$.

A crucial observation is that Equation (16.1.8) must be true for *all* values of z. This fact can only be true if the coefficients of each power of $z - 1$ vanishes separately, i.e. if

$$0 = [c_{n+1}\,(n+1) - A\,c_n] \tag{16.1.9}$$

for every value of n. This relationship is called a *recurrence relation*. You can use it to find values of the coefficients for high values of n if you know the coefficients for lower values of n. Solve for c_{n+1}:

$$c_{n+1} = \frac{A}{n+1}\,c_n \tag{16.1.10}$$

By keeping c_0 as an unknown constant, we can find other coefficients c_n by an iterative process.

$$c_1 = \frac{A}{1}\,c_0 \tag{16.1.11}$$

$$c_2 = \frac{A}{2}\,c_1 = \frac{A^2}{(2)(1)}\,c_0 \tag{16.1.12}$$

$$c_3 = \frac{A}{3}\,c_2 = \frac{A^3}{(3)(2)(1)}\,c_0 \tag{16.1.13}$$

$$c_4 = \frac{A}{4}\,c_3 = \frac{A^4}{(4)(2)(1)}\,c_0 \tag{16.1.14}$$

$$\vdots \tag{16.1.15}$$

$$c_n = \frac{A}{n}\,c_n = \frac{A^n}{n!}\,c_0 \tag{16.1.16}$$

In this case, we are able to see what the formula will be for the generic value of c_n. In most cases, this we will *not* be able to determine the general formula and will be forced to trucate the series when we have as many terms of the series as we need for the accuracy that we care about.

Our final answer is:

$$\begin{aligned} f(x) &= c_0(1 + \frac{A}{1!}(z-1) + \frac{A^2}{2!}(z-1)^2 + \cdots + \frac{A^n}{n!}(z-1)^n + \dots) \\ &= c_0 \sum_{n=0}^{\infty} \frac{A^n}{n!}(z-1)^n \\ &= c_0 e^{A(z-1)} \end{aligned}$$

Since we are solving a first order differential equation, we expect a single solution multiplied by an overall arbitrary constant. Notice that the coefficient of the first term in the series c_0, through the recurrence relation, becomes a factor in every term and therefore becomes the overall arbitrary constant.

For an nth order equation, we expect to get n linearly independent solutions using this method. In exceptional cases, the extra solutions will be a power series multiplied by a logarithm. The technical theorems that delineate when you can expect solutions can be found in Section 16.3.

16.2 Series Solutions of Legendre's Equation

Definition 16.2.1 Legendre's Equation. Legendre's equation is

$$\left((1-z^2)\frac{\partial^2}{\partial z^2} - 2z\frac{\partial}{\partial z} - A\right) P(z) = 0 \tag{16.2.1}$$

It arises during the separation of variables procedure for any PDE involving the Laplacian in spherical coordinates, see Section 18.5. ♢

In this section, we will use series methods to find the general solution of (16.2.1). Assume that the solution can be written as a power series

$$P(z) = \sum_{n=0}^{\infty} a_n z^n \tag{16.2.2}$$

Then we have

$$\frac{dP}{dz} = \sum_{n=0}^{\infty} a_n n z^{n-1} \tag{16.2.3}$$

$$\frac{d^2P}{dz^2} = \sum_{n=0}^{\infty} a_n n(n-1) z^{n-2} \tag{16.2.4}$$

Our job is to solve for the unknown coefficients a_n.

Plug (16.2.2)–(16.2.4) into (16.2.1) to obtain

$$\begin{aligned} 0 = &\sum_{n=0}^{\infty} a_n n(n-1) z^{n-2} - z^2 \sum_{n=0}^{\infty} a_n n(n-1) z^{n-2} \\ &- 2z \sum_{n=0}^{\infty} a_n n z^{n-1} - A \sum_{n=0}^{\infty} a_n z^n \end{aligned} \tag{16.2.5}$$

The next step is to get the power of the independent variable z to be the same in each term of (16.2.5). In the last three terms, the power is z^n. (Don't forget the powers of z in front of the sum sign.) But in the first term, the power is z^{n-2}. Since the summation variable n is a dummy variable (just like

a dummy variable of integration), we can shift $n \to n+2$ in the first term only, i.e.

$$\text{First Term} = \sum_{n=0}^{\infty} a_n\, n(n-1)\, z^{n-2} \tag{16.2.6}$$

$$\begin{aligned}
&= \sum_{n=-2}^{\infty} a_{n+2}\,(n+2)(n+1)\, z^n \\
&= a_0 \cancelto{0}{(-2+2)}(-2+1)\, z^{-2} \\
&\qquad + a_1(-1+2)\cancelto{0}{(-1+1)}\, z^{-1} \\
&\qquad + \sum_{n=0}^{\infty} a_{n+2}\,(n+2)(n+1)\, z^n \\
&= \sum_{n=0}^{\infty} a_{n+2}\,(n+2)(n+1)\, z^n
\end{aligned} \tag{16.2.7}$$

Pay special attention to what happened to the lower limit of the sum. After the index is shifted, sum would start at $n=-2$, but the factor of $(n+2)$ in the first term and the factor of $(n+1)$ in the second term mean that these terms are zero and we can eliminate them from the sum. This cancellation doesn't always happen, you should check. If it doesn't happen, you just need to carry the extra terms through to the end of the calculation.

Plug (16.2.7) into (16.2.5). At the same time, bring any overall factors of z into the corresponding sums. Finally, since each sum now has a factor of z^n and runs over the same range, group the sums together.

$$\begin{aligned}
&\sum_{n=0}^{\infty} a_{n+2}\,(n+2)(n+1)\, z^n - \sum_{n=0}^{\infty} a_n\, n(n-1)\, z^n \\
&\qquad - 2\sum_{n=0}^{\infty} a_n\, n\, z^n - A\sum_{n=0}^{\infty} a_n\, z^n
\end{aligned} \tag{16.2.8}$$

$$= \sum_{n=0}^{\infty} \left[a_{n+2}\,(n+2)(n+1) - a_n\,(n(n-1) + 2\,n + A)\right] z^n \tag{16.2.9}$$

Now comes the MAGIC part. Since (16.2.9) is true *for all values of* z, the coefficient of z^n for each term in the sum (i.e. the quantity in square brackets) must separately be zero, i.e.

$$0 = a_{n+2}\,(n+2)(n+1) - a_n\,(n(n-1) + 2\,n + A). \tag{16.2.10}$$

Definition 16.2.2 Recurrence Relation. We can solve for a_{n+2} in terms of a_n to obtain the **recurrence relation** which relates coefficients in the power series to coefficients with smaller values of a_n

$$a_{n+2} = \frac{n(n+1)+A}{(n+2)(n+1)}\, a_n. \tag{16.2.11}$$

◊

By plugging successive even values of n into the recurrence relation (16.2.11), usining an iterative process, allows us to find a_2, a_4, etc. in terms of the arbitrary constant a_0 and successive odd values of n allow us to find a_3,

a_5, etc. in terms of the arbitrary constant a_1. Thus, for the second-order differential equation (16.2.1), we obtain two solutions as expected. a_0 becomes the normalization constant for a solution with only even powers of z and a_1 becomes the normalization constant for a solution with only odd powers of z. For example:

$$a_2 = \frac{A}{2}a_0 \tag{16.2.12}$$

$$a_4 = \frac{6+A}{12}a_2 = \left(\frac{6+A}{12}\right)\left(\frac{A}{2}\right)a_0 \tag{16.2.13}$$

$$\vdots$$

$$a_3 = \frac{2+A}{6}a_1 \tag{16.2.14}$$

$$a_5 = \frac{12+A}{20}a_3 = \left(\frac{12+A}{20}\right)\left(\frac{2+A}{6}\right)a_1 \tag{16.2.15}$$

$$\vdots$$

Don't forget to plug these coefficients back into the original power series anzatz (16.2.2). It is rare to be able to find a closed form expression for general n, so you may only be finding an approximation to a solution, but you can keep as many terms as you have patience to calculate.

$$\begin{aligned} P(z) = a_0 &\left[\frac{A}{2}z^0 + \left(\frac{6+A}{12}\right)\left(\frac{A}{2}\right)z^2 + ...\right] \\ + \quad a_1 &\left[\frac{2+A}{6}z^1 + \left(\frac{12+A}{20}\right)\left(\frac{2+A}{6}\right)z^3 + ...\right] \end{aligned} \tag{16.2.16}$$

In general, the solutions of an ordinary linear differential equation can blow-up only where the coefficients of the equation itself are singular, in this case at $z = \pm 1$ (which correspond to the north and south poles $\theta = 0, \pi$ of spherical coordinates). But there is nothing special about physics at these points, only the choice of coordinates is special there. Therefore, in physics contexts, we may want to choose solutions of (16.2.1) which are regular (non-infinite) at $z = \pm 1$. This is an important example of a problem where the choice of coordinates for a partial differential equation end up imposing boundary conditions on the ordinary differential equation which comes from it. Therefore, the infinite series (16.2.2) will typically blow up at the endpoints $z = \pm 1$, but a polynomial can not. So if we choose the special values for the separation constant A to be $A = -\ell(\ell+1)$ where ℓ is a non-negative integer, we see from (16.2.11) that for $n \geq \ell$ the coefficients become zero and one of the series terminates in a polynomial.

Definition 16.2.3 Legendre Polynomials. The solutions of Legendre's equation for $A - \ell(\ell+1)$ are polynomials of degree ℓ, denoted P_ℓ, and called **Legendre polynomials**. ◊

16.3 Power Series Solutions: Definitions and Theorems

In this section, we will briefly discuss the theorems that state when a *second order* linear ODE has power series solutions.

First, write the ode in the special form

$$y'' + p(z)y' + q(z)y = 0. \tag{16.3.1}$$

Note the coefficient one in front of the second derivative. Now exampine the functions $p(z)$ and $q(z)$, thought of as functions of the complex variable z.

Definition 16.3.1 Regular Point of an ODE. If $p(z)$ and $q(z)$ are *analytic* at a point $z = z_0$, the z_0 is said to be a **regular point of the differential equation**. (The word *analytic* is a technical term for a complex-valued function which is (complex) differentiable at the point. You can learn more about this concept online. But for practical purposes, it means that the function does not blow up at the point z_0, nor is it otherwise badly behaved, e.g. the origin of a square root.) ◊

Theorem 16.3.2 *If the coefficients $p(z)$ and $q(z)$ are analytic at a point z_0, then a power series solution of the differential equation (16.3.1), expanded around the point z_0 exists, and furthermore, the radius of convergence for the series extends at least as far as the nearest singularity (point of non-analyticity) of $p(z)$ or $q(z)$ in the complex plane. Usually, there will be two such power series solutions, but sometimes the second solution will be a power series times a logarithm.*

Definition 16.3.3 Regular Singularity of an ODE. If $(z - z_0)p(z)$ and $(z - z_0)^2 q(z)$ are analytic, then the point z_0 is called a **regular singular point** or **regular singularity**. ◊

Theorem 16.3.4 *Theorem: If z_0 is a regular singular point then equation (16.3.1) can be solved by an extension of power series methods called a* Frobenius Series*. The solution will consist of: (1) two Frobenius series, or (2) one Frobenius series $y_1(z - z_0)$ and a second solution $y_2(z - z_0) = y_1(z - z_0)\ln(z - z_0) + y_0(z - z_0)$, where $y_0(z - z_0)$ is a second Frobenius series.*

We will not discuss this method further here, but you can look it up online or in a more comprehensive mathematical methods text, if necessary.

Chapter 17

Step and Delta Functions

17.1 Kronecker Delta

Definition 17.1.1 The Kronecker Delta. The **Kronecker Delta** is a simple switch that compares two values i and j in some discrete set. The switch turns on when i is the same as j and off when they are different, i.e.,

$$\delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \tag{17.1.1}$$

$\Diamond$

Example 1: Kronecker Delta in a Sum. The most common place that the Kronecker delta appears is inside a sum. In this case, it can be used to collapse the sum to a single term. For example:

$$\sum_{i=1}^{\infty} a_i \, \delta_{i3} = a_1 \cancelto{0}{\delta_{13}} + a_2 \cancelto{0}{\delta_{23}} + a_3 \cancelto{1}{\delta_{33}} + \ldots \tag{17.1.2}$$

$$= a_3 \tag{17.1.3}$$

In this example the factor of δ_{i3} is zero in every term except the one when $i = 3$, so all of those terms are zero and do not contribute to the sum. When $i = 3$, the factor of δ_{i3} is just one, so that is the only term that contributes.

Example 2: Trace of a Matrix with Kronecker Deltas. If you want to add up all of the elements a_{ij} of a matrix A (where, by convention, the first index i labels the rows and the second index j labels the columns), this requires a double sum, one for each index.

$$\sum_{i=1}^{3} \sum_{i=j}^{3} a_{ij} \tag{17.1.4}$$

If, instead, you want to find the trace of the matrix $\mathrm{tr}A$, then you only want to add up the diagonal elements. A Kronecker delta in the double sum will ensure that you only take the elements for which the row and column labels are the same.

$$\mathrm{tr}A \doteq \sum_{i=1}^{3} \sum_{i=j}^{3} a_{ij}\delta_{ij} \tag{17.1.5}$$

$$= \sum_{i=1}^{3} a_{ii} \tag{17.1.6}$$

Question 17.1.2 Try it yourself: The Identity Matrix. *Write the elements of the* 3×3 *identity matrix in terms of the Kronecker delta.*

$$I \doteq \begin{pmatrix} \delta_{11} & \delta_{12} & \delta_{13} \\ \delta_{21} & \delta_{22} & \delta_{23} \\ \delta_{31} & \delta_{32} & \delta_{33} \end{pmatrix} \tag{17.1.7}$$

17.2 Step and Delta Function Motivation

Consider a mass sliding along a frictionless surface. It collides, elastically, with a wall. The velocity of the mass as a function of time is shown in Figure 17.2.1 and its acceleration is shown in Figure 17.2.2.

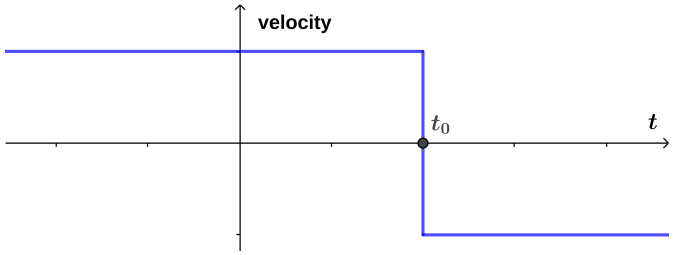


Figure 17.2.1 The velocity of an idealized mass colliding with a wall.

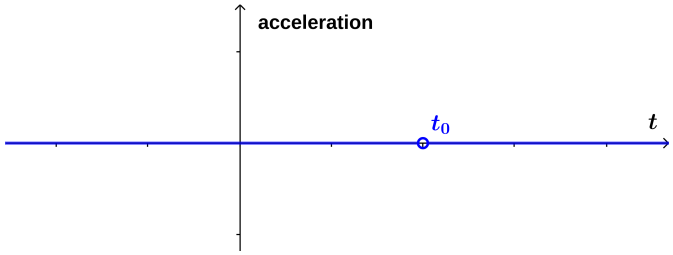


Figure 17.2.2 The acceleration of an idealized mass colliding with a wall.

Clearly, this is a highly idealized situation. In the real world, the mass will slow down slightly due to a small amount of friction, the interaction with the wall will not be instantaneous, nor will it be completely elastic, and the rebound will be somewhat slower than the speed when the mass hits the wall, etc. But suppose these differences from ideal are very small compared to the motion itself and that we do not care about the details, only the overall qualitative behavior. Then, we can model the behavior with two new functions, the step function (defined in Section 17.3) and the delta function (defined in Section 17.4). These functions are really easy to work with in algebra and calculus settings. With a little bit of effort now, you will come to welcome them in your work.

The tricky part, of course, is what happens at the moment (labelled t_0 in the figures) that the mass hits the wall. All of the complications of the motion are compressed into that one time. The velocity changes *instantaneously* from its initial value $v_0\,\hat{x}$ to $-v_0\,\hat{x}$. This behavior will be modeled by the step function.

Even worse, is the acceleration. The acceleration is the derivative of the velocity with respect to time, so the acceleration is zero before the mass hits the wall and after the mass hits the wall. But what is the value of the acceleration

at the moment the mass hits the wall? Clearly, the acceleration is infinite. The delta function is what allows us to specify exactly how big this infinity is, so that the velocity by the correct amount.

17.3 Step Functions

Definition 17.3.1 The Step or Heaviside Function. The **step function** $\Theta(x)$, also called the **Heaviside function** or **theta function**, is defined to be 0 if $x < 0$ and 1 if $x > 0$. See Figure 17.3.2. A function that behaves differently in two or more different regions is called **piecewise** and often written

$$\Theta(x) = \begin{cases} 0 & x < 0 \\ \frac{1}{2} & x = 0 \\ 1 & x > 0 \end{cases} \tag{17.3.1}$$

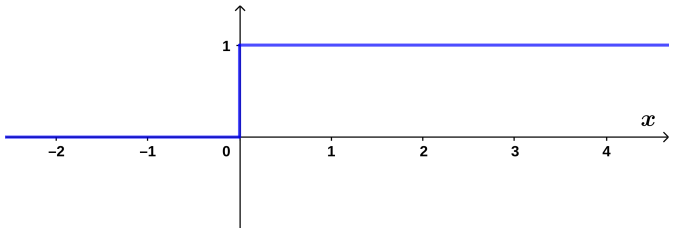


Figure 17.3.2 The step function $\Theta(x)$.

◊

In most physical problems, it is unnecessary to know the exact value of $\Theta(x)$ at the discontinuity. If it ever matters, it is usually easiest to define it symmetrically, i.e.

$$\Theta(0) = \frac{1}{2}. \tag{17.3.2}$$

Step functions are used to model idealized physical situations where some quantity changes rapidly from one value to another in such a way that the exact details of the change are irrelevant for the solution of the problem, e.g. edges of materials or a process that switches on abruptly at a particular time, etc.

By shifting the argument of the function, it is possible to put the discontinuity of the theta function wherever we need it. In Figure 17.3.3 you can see that the graph of $\Theta(x-2)$ has discontinuity at $x = 2$, instead of at $x = 0$.

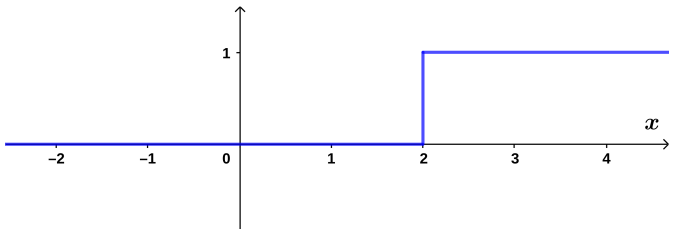


Figure 17.3.3 The function $\Theta(x-2)$.

Most often the step function appears in contexts where it is multiplying some other function $f(x)$. In this case, the step function can be thought of as a switch, that "turns on" the function $f(x)$. You can watch the operation of the switch in Figure 17.3.4 below.

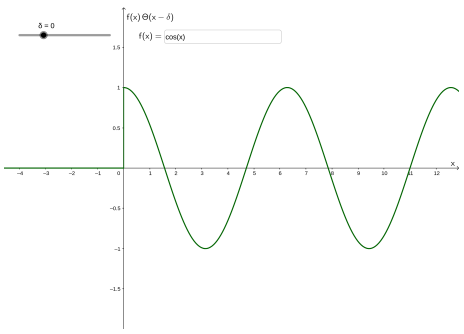


Figure 17.3.4 An applet that allows you to change the value of δ in $f(x)\,\Theta(x-\delta)$. The default function displayed is $f(x)=\cos(x)$.

The step function can also be used to turn a function off, since

$$\Theta(-x) = 1 - \Theta(x) \tag{17.3.3}$$

is a step down, rather than up.

Sensemaking 17.3.1 Try It Yourself: Graphing Step Functions. Make sure that you are able to graph all of the following functions:

$$\begin{aligned}
&f(x) = 2\Theta(x),\\
&f(x) = \Theta(x-2),\\
&f(x) = \Theta(2x-3),\\
&f(x) = \Theta(2-x),\\
&f(x) = \Theta(x)\,\Theta(x-2),\\
&f(x) = \Theta(x) - \Theta(x-2),\\
&f(x) = \sin x\,\Theta(x-\frac{\pi}{2}).
\end{aligned}$$

17.4 The Dirac Delta Function

Definition 17.4.1 The Dirac Delta Function.

Technically, the delta function is not really a function. It is a mathematical entity called a "distribution" which is well defined only when it appears under an integral sign, as in (17.4.2).

The **Dirac delta function** $\delta(x)$ has has the following defining properties:

$$\delta(x) = \begin{cases} 0 & x \neq 0 \\ \infty & x = 0 \end{cases} \tag{17.4.1}$$

$$\int_b^c \delta(x)\,dx = 1 \qquad\qquad b < 0 < c \tag{17.4.2}$$

$$x\,\delta(x) \equiv 0. \tag{17.4.3}$$

$\Diamond$

Using the Dirac Delta Function in an Integral. The properties of the delta function allow us to compute

$$\int_{-\infty}^{\infty} f(x)\,\delta(x)\,dx = \int_{-\infty}^{\infty} f(0)\,\delta(x)\,dx$$

$$= f(0) \int_{-\infty}^{\infty} \delta(x)\, dx$$
$$= f(0)$$

In the first equality, it is safe to replace the function $f(x)$ with its value $f(0)$ at $x = 0$ since everywhere else the integrand is zero, due to the delta function.

We can shift the "spike" in the delta function as usual, obtaining $\delta(x - a)$. This shifted delta function satisfies

$$\int_{-\infty}^{\infty} f(x)\, \delta(x - a)\, dx = f(a) \tag{17.4.4}$$

To Remember. The Dirac delta function can be used inside an integral to pick out the value of a function at any desired point.

17.5 Relationship between Delta and Step Functions

The Dirac Delta and Step Functions are a Derivative/Integral Pair. We can relate the delta function to the step function in the following way. Consider the integral

$$\int_{-\infty}^{x} \delta(u - a)\, du \tag{17.5.1}$$

Notice the variable x in the upper limit of the integral. The value of this integral is 0 if we stop integrating before we reach the peak of the delta function, i.e. for $x < a$. If we integrate through the peak, the value of the integral is 1, i.e. for $x > a$. Thus, we have argued that the value of the integral, thought of as a function of x, is just the step function

$$\Theta(x - a) = \int_{-\infty}^{x} \delta(u - a)\, du \tag{17.5.2}$$

(Recall that we don't really care about the choice of $\Theta(0)$, so we don't need to worry about the value of this function if we stop integrating exactly at $x = a$.)

If the step function is the integral of the delta function, then the delta function must be the derivative of the step function.

$$\frac{d}{dx}\Theta(x - a) = \delta(x - a) \tag{17.5.3}$$

You should be able to persuade yourself that this statement is reasonable geometrically if you think of the derivative of a function as representing its slope.

Sensemaking 17.5.1 The derivative of the step function. Prove that the derivative of the step function is the delta function, i.e. prove Equation (17.5.3).

Solution. We need to show that

$$\int_{b}^{c} f(x)\, \delta(x - a)\, dx = f(a) \tag{17.5.4}$$

for $b < a < c$, where

$$\delta(x - a) = \frac{d}{dx}\, \Theta(x - a) \tag{17.5.5}$$

The main strategy is to use integration by parts, paying strict attention to the limits of integration.

$$\begin{aligned}
\int_b^c f(x)\,\delta(x-a)\,dx &= \int_b^c f(x)\,\frac{d}{dx}\,\Theta(x-a)\,dx \\
&= f(x)\,\Theta(x-a)\big|_b^c - \int_b^c \frac{d}{dx}(f(x))\,\Theta(x-a)\,dx \\
&= \{f(c)-0\} - \int_a^c \frac{d}{dx}(f(x))\,dx \\
&= f(c) - \{f(x)\big|_a^c\} \\
&= f(c) - \{f(c)-f(a)\} \\
&= f(a)
\end{aligned}$$

17.6 Compare Kronecker and Dirac Deltas

Comparing the Kronecker and Dirac Deltas. In Section 17.1, we defined the Kronecker delta as

$$\delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

In Section 17.4, we defined the Dirac delta as

$$\delta(x-a) = \begin{cases} 0 & x \neq 0 \\ \infty & x = a \end{cases}$$

These definitions look very much the same. What is the difference?

One difference comes from the input variables (the domain). For the Kronecker delta, the input variables i and j are discrete variables; for the Dirac delta, the input variable x is a continuous variable. You should always choose to use the form of the delta that is appropriate for the input variables.

Definition 17.6.1 Discrete vs. Continuous Variables. A variable is called a **continuous variable** if for any two values you can always find another in between them (think about the real numbers). The values of these variables are typically obtained by measuring; common examples are distance and time. If the values of the variable are spaced apart (think about the integers), so that there is always a gap between one value and its nearest neighbor(s), the variable is called a **discrete variable**. These values of these variables are typically obtained by counting; simple examples include the sets $\{0,1,2,3\}$ and the even integers. These variables can be either finite or countably infinite. Examples can also include more abstract sets such as $\{x,y,z\}$ since the elements could be assigned discrete numbers according to their position in the list. ♢

Another difference between the Kronecker delta and the Dirac delta comes from the output variables (the range). The Kronecker delta compares the discrete input variables i and j. It takes the value one whenever these two input variables are the same. The Dirac delta compares the continuous input variable x to the constant parameter a. It takes the value ∞ whenever x is the same a a. This choice between one and ∞ comes from the ways in which the deltas are used. The Kronecker delta is used to pick out a particular term in a

sum (see Section 17.1). For example, if we want to pick out the term a_N in a sum, we use δ_{iN}

$$\sum_{i=1}^{\infty} a_i \, \delta_{iN} = a_N$$

On the other hand, the Dirac delta is used to pick out a particular term in an *integral* (see Section 17.4). For example, if we want to pick out the value of the function $f(x)$ when $x = a$ in an integral, we use $\delta(x - a)$

$$\int_{-\infty}^{\infty} f(x) \, \delta(x - a) \, dx = f(a)$$

Visualization of the Delta Function. To understand why the delta function under an integral sign picks out a particular value of the integrand, it may help to think of the delta function as the limit of a sequence of steps $\delta_\epsilon(x)$, Each step is narrower (width 2ϵ) and higher (height $1/(2\epsilon)$) than the previous step, such that the area under each step is always one; see Figure Figure 17.6.2.

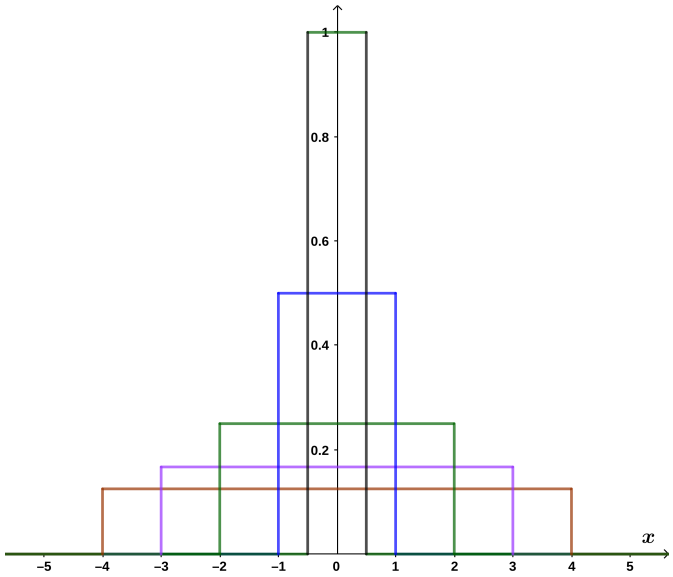


Figure 17.6.2 The function $\delta(x)$ can be approximated by a series of steps that get progressively thinner and higher in such a way that the area under the curve is always equal to one.

Then

$$\int_{-\infty}^{\infty} f(x) \, \delta_\epsilon(x - a) \, dx \tag{17.6.1}$$

give the average value of $f(x)$ on the interval determined by ϵ. In the limit that ϵ becomes infinitesimally small, then the peak becomes infinitely narrow and infinitely high in just the right way to pick out the value of the function at $x = a$.

17.7 Dimensions of Step and Delta Functions

Dimensions of the Step Function. The definition of the step function, (17.3.1), i.e.

$$\Theta(x) = \begin{cases} 0 & x < 0 \\ \frac{1}{2} & x = 0 \\ 1 & x > 0 \end{cases}$$

clearly shows that the value of the step function is either the pure number zero or one, with no dimensions.

In Figure 17.3.4, you saw a figure where the step function was multiplied by some other function $f(x)$ so that the step function could be thought of as a switch, that "turns on" the function $f(x)$. In this case, the product function $f(x)\,\Theta(x)$ inherits the dimensions of $f(x)$.

Dimensions of the Delta Function. In contrast to the step function, above, the delta function *does* have dimensions, but the dimensions change, according to the context. They are determined by the defining equation (17.4.2), i.e.

$$\int_b^c \delta(x)\,dx = 1 \qquad\qquad b < 0 < c$$

Since we can think of the differential dx as a little piece of x, it has the same dimensions as x. The integral says to add up a bunch of little pieces that look like $\delta(x)\,dx$ and end up with the dimensionless number one. That tells us that the delta function $\delta(x)$ by itself has dimensions that are the inverse of the dimensions of dx. For example, if x has dimensions of length L, then $\delta(x)$ has dimensions of inverse length L^{-1}.

17.8 Properties of the Dirac Delta Function

There are many properties of the delta function which follow from the defining properties in Section 17.4. Some of these are:

$$\begin{aligned}
\delta(x) &= \delta(-x) \\
\frac{d}{dx}\,\delta(x) &= -\frac{d}{dx}\,\delta(-x) \\
\int_b^c f(x)\,\delta'(x-a)\,dx &= -f'(a) \\
\delta(ax) &= \frac{1}{|a|}\,\delta(x) \\
\delta\big(g(x)\big) &= \sum_i \frac{1}{|g'(x_i)|}\,\delta(x-x_i) \\
\delta(x^2-a^2) &= |2a|^{-1}\,[\delta(x-a)+\delta(x+a)] \\
\delta\big((x-a)(x-b)\big) &= \frac{1}{|a-b|}\,[\delta(x-a)+\delta(x-b)]
\end{aligned}$$

where a and b are real-valued constants and the function $g(x)$ has zeros at x_i with properties $g(x_i) = 0$ and $g'(x_i) \neq 0$. The first two properties show that the delta function is even and its derivative is odd.

Sensemaking 17.8.1 Prove properties of the delta function. Prove some or all of the properties of the Dirac delta function listed in Section 17.8.

17.9 Representations of the Dirac Delta Function

Some other useful representations of the delta function are:

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ixt}\,dt$$
$$\delta(x) = \lim_{\epsilon\to 0}\frac{1}{2\epsilon}\left[\Theta(x+\epsilon)-\Theta(x-\epsilon)\right]$$
$$\delta(x) = \lim_{\epsilon\to 0}\frac{1}{\sqrt{2\pi}\,\epsilon}\exp\left(-\frac{x^2}{2\epsilon^2}\right)$$
$$\delta(x) = \frac{1}{\pi}\lim_{\epsilon\to 0}\frac{\epsilon}{x^2+\epsilon^2}$$
$$\delta(x) = \lim_{N\to\infty}\frac{\sin Nx}{\pi x}$$
$$\delta(x) = \frac{1}{2}\frac{d^2}{dx^2}|x|$$
$$\delta(x) = \frac{1}{\pi^2}\int_{-\infty}^{\infty}\frac{dt}{t(t-x)}$$

where Cauchy-Principal Value integration is implied in the last integral. (You can find more limit representations of the delta function at the Wolfram Research Site[1]).

In quantum mechanics, we sometimes use the closure relation given by:

$$\delta(x-x') = \sum_{n=0}^{\infty}\phi_n^*(x)\,\phi_n(x')$$

where the ϕ_n are any complete set of orthonormal eigenfunctions for a hermitian differential operator.

17.10 The Dirac Delta Function in Three Dimensions

The three-dimensional delta function must satisfy:

$$\int_{all\ space}\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}_0)\,d\tau = 1 \tag{17.10.1}$$

where $\vec{\boldsymbol{r}} = x\,\hat{\boldsymbol{x}} + y\,\hat{\boldsymbol{y}} + z\,\hat{\boldsymbol{z}}$ is the position vector and $\vec{\boldsymbol{r}}_0 = x_0\,\hat{\boldsymbol{x}} + y_0\,\hat{\boldsymbol{y}} + z_0\,\hat{\boldsymbol{z}}$ is the position at which the "peak" of the delta function occurs. In rectangular coordinates, it is just the product of three one-dimensional delta functions:

$$\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}_0) = \delta(x-x_0)\,\delta(y-y_0)\,\delta(z-z_0) \tag{17.10.2}$$

so that:

$$\int_{all\ space}\delta^3(\vec{\boldsymbol{r}})\,d\tau = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\delta(x)\,\delta(y)\,\delta(z)\,dx\,dy\,dz = 1 \tag{17.10.3}$$

But in curvilinear coordinates, with $d\tau = h_u h_v h_w\,du\,dv\,dw$, it has a Jacobian in it. Thus,

$$\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}_0) \neq \delta(u-u_0)\,\delta(v-v_0)\,\delta(w-w_0) \tag{17.10.4}$$

[1] functions.wolfram.com/GeneralizedFunctions/DiracDelta/09/

but instead:

$$\delta^3(\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_0) = \frac{1}{h_u h_v h_w}\delta(u - u_0)\,\delta(v - v_0)\,\delta(w - w_0) \tag{17.10.5}$$

In particular, in cylindrical coordinates:

$$\delta^3(\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_0) = \frac{1}{r}\delta(r - r_0)\,\delta(\theta - \theta_0)\,\delta(z - z_0) \tag{17.10.6}$$

and in spherical coordinates:

$$\delta^3(\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_0) = \frac{1}{r^2\sin(\theta)}\delta(r - r_0)\,\delta(\theta - \theta_0)\,\delta(\phi - \phi_0) \tag{17.10.7}$$

Just as with the delta function in one dimension, when the three-dimensional delta function is part of an integrand, the integral just picks out the value of the rest of the integrand at the point where the delta function has its peak.

$$\int\limits_{\text{all space}} f(\vec{\boldsymbol{r}})\,\delta^3(\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}_0)\,d\tau = f(\vec{\boldsymbol{r}}_0) \tag{17.10.8}$$

17.11 The Exponential Representation of the Dirac Delta Function

As mentioned in Section 17.9, the Dirac delta function can be written in the form

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\,dk, \tag{17.11.1}$$

or more generally,

$$\delta(x - x_0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x-x_0)}\,dk. \tag{17.11.2}$$

We outline here the derivation of this representation.

In order to evaluate the integral, we introduce a regularization factor, $e^{-k\epsilon}$, as follows:

$$\begin{aligned}
\int_{-\infty}^{\infty} e^{ikx}\,dk &= \int_{-\infty}^{0} e^{ikx}\,dk + \int_{0}^{\infty} e^{ikx}\,dk \\
&= \int_{0}^{\infty} e^{-ikx}\,dk + \int_{0}^{\infty} e^{ikx}\,dk \\
&= \int_{0}^{\infty} (e^{ikx} + e^{-ikx})\,dk \\
&= \lim_{\epsilon\to 0^+}\int_{0}^{\infty} (e^{ikx} + e^{-ikx})\,e^{-k\epsilon}\,dk \\
&= \lim_{\epsilon\to 0^+}\int_{0}^{\infty} (e^{ik(x+i\epsilon)} + e^{-ik(x-i\epsilon)})\,dk \\
&= \lim_{\epsilon\to 0^+}\left[\frac{e^{ik(x+i\epsilon)}}{i(x+i\epsilon)} + \frac{e^{-ik(x-i\epsilon)}}{-i(x-i\epsilon)}\right]_0^{\infty} \\
&= \lim_{\epsilon\to 0^+}\left(0 + 0 - \frac{1}{i(x+i\epsilon)} - \frac{1}{-i(x-i\epsilon)}\right)
\end{aligned}$$

$$= \lim_{\epsilon \to 0^+} \left(\frac{i}{x + i\epsilon} - \frac{i}{x - i\epsilon} \right)$$
$$= \lim_{\epsilon \to 0^+} \frac{2\epsilon}{x^2 + \epsilon^2} = \begin{cases} 0 & x \neq 0 \\ \infty & x = 0 \end{cases}$$

where we have used the fact that, for $\epsilon > 0$, $e^{-k\epsilon}$ goes to 0 as k goes to ∞.[1]

It remains to show that the final expression has the correct normalization. But

$$\int_{-\infty}^{\infty} \frac{2\epsilon}{x^2 + \epsilon^2}\, dx = 2 \arctan\left(\frac{x}{\epsilon}\right) \Bigg|_{-\infty}^{\infty} = 2\pi, \tag{17.11.3}$$

which is independent of ϵ, so taking the limit is trivial.

[1] The use of such regularization factors is quite common. Rigorous mathematical justification can be given, but informal arguments along the lines above are usually sufficient—if the informal argument works, the formal derivation should also, for an appropriate, reasonable class of functions.

Chapter 18

Partial Differential Equations

18.1 Important PDEs in Physics

On this page you will find a list of most of the important PDEs in physics with their names. Notice that the spatial derivatives always comes in the form of the laplacian ∇^2. This particular spatial dependence occurs in physics PDEs because space is rotationally invariant. Also notice that some of the equation have no time derivatives, some have a first order time derivative, and some have a second order time derivative. This difference is the foundation of an important classification scheme (see Section 18.2) and also affects what kinds of initial conditions are appropriate to guarantee that a unique solution exists (see Section 18.3).

Names and forms for important partial differential equations in physics.
Laplace's Equation:

Many time-independent problems are described by *Laplace's equation*. This is defined for $\psi = \psi(x, y, z)$ by:

$$\nabla^2\psi = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = 0. \tag{18.1.1}$$

The differential operator, ∇^2, defined by eq.(1) is called the *Laplacian* operator, or just the *Laplacian* for short. Some examples of Laplace's equation are the electrostatic potential in a charge-free region, the gravitational potential in a matter-free region, the steady-state temperature in a region with no heat source, the velocity potential for an incompressible fluid in a region with no vortices and no sources or sinks.

Poisson's Equation:

Poisson's equation is like Laplace's equation except that it allows an inhomogeneous term, $f(x, y, z)$, known as the source density. It has the form:

$$\nabla^2\psi = f(x, y, z) \tag{18.1.2}$$

Schrödinger's Equation:

A great deal of non-relativistic quantum mechanics is devoted to the study of the solutions to the *time-dependent Schrödinger equation*:

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V(x, y, z)\psi. \tag{18.1.3}$$

This equation governs the time dependence of the wave-function of a particle moving in a given potential, $V(x, y, z)$. A special role is played by solutions

to (4) that have the simple form: $\psi = \phi(x, y, z)\exp(-iEt/\hbar)$. The function ϕ satisfies the *time-independent Schrödinger equation* or, more correctly, the *Schrödinger (or energy) eigenvalue equation*:

$$-\frac{\hbar^2}{2m}\nabla^2\phi + V(x, y, z)\phi = E\phi. \tag{18.1.4}$$

In both of these equations $\hbar$ and m represent real constants. E is a constant that emerges during the separation of variables procedure. i, as usual, satisfies $i^2 = -1$.

The Diffusion Equation:

The pde governing the concentration of a diffusing substance or the non-steady-state temperature in a region with no heat sources is the *diffusion equation*:

$$\frac{\partial\psi}{\partial t} - \kappa\nabla^2\psi = 0. \tag{18.1.5}$$

κ is a real constant called the *diffusivity*.

The Wave Equation:

Wave propagation, including waves on strings or membranes, pressure waves in gasses, liquids or solids, electromagnetic waves and gravitational waves, and the current or potential along a transmission line all satisfy the following *wave equation*:

$$-\frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} + \nabla^2\psi = 0. \tag{18.1.6}$$

The real constant v can be interpreted as the speed of the corresponding wave.

The Klein-Gordon Equation:

Disturbances traveling through fields that mediate forces with a finite range, satisfy a modification of the wave equation called the *Klein-Gordon equation*. It is given by:

$$-\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} + \nabla^2\psi + \frac{m^2c^2}{\hbar^2}\psi = 0. \tag{18.1.7}$$

The coefficients c, $\hbar$ and m all represent constants.

Helmholtz's Equation:

The equation:

$$\nabla^2\psi + k^2\psi = 0 \tag{18.1.8}$$

is known as *Helmholtz's equation* and arises as the time-independent part of the diffusion or wave equations. k is a constant that emerges during the separation of variables procedure.

18.2 Classification of PDEs

18.2.1 Why do you want to classify solutions?

If we can classify a PDE that we are trying to solve, according to the scheme given below, it will help us extend qualitative knowledge that we have about the nature of solutions of similar PDEs to the current case. Most importantly, the types of initial conditions that are needed to ensure that the solution is unique vary according to the classification–see Section 18.3.

In physics situations, the classification is usually obvious: if there are two time derivatives, the equation is hyperbolic and we will need two initial conditions on the entire spatial region to make the solution unique; if there is only a single time derivative, the equation is parabolic and we will need only a

single initial condition; if the equation has no time derivatives, the equation is elliptic and the solutions are qualitatively different from the previous two cases. You should look at the important PDEs in physics listed in Section 18.1 and classify each one.

If you want to see the formal mathematics for the classification (optional), read on:

18.2.2 Form of the equation

The most general 2nd order, linear, PDE can be written:

$$\mathcal{L}\psi = b \tag{18.2.1}$$

where

$$\mathcal{L}\psi = \sum_{i,j=1}^{4} A_{ij}(x_k)\frac{\partial^2\psi}{\partial x_i \partial x_j} + \sum_{i=1}^{4} B_i(x_k)\frac{\partial\psi}{\partial x_i} + C(x_k)\psi \tag{18.2.2}$$

and $b(x_k)$ is a source term which may depend on the spatial variables (x_k).

18.2.3 Optional Mathematical Details of the Classification Scheme

The PDE is classified according to the signs of the eigenvalues $\lambda_i(x_k)$ of the matrix of functions $A_{ij}(x_k)$.

1. *Elliptic:* $\lambda_i(x_k)$ are nowhere vanishing. All have the same sign. Ex: Poisson, Laplace, Helmholtz

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{18.2.3}$$

$$A_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{18.2.4}$$

2. *Parabolic:* One eigenvalue vanishes everywhere (usually time dependence), the others are nowhere vanishing and have the same sign. Ex: Diffusion, Schroedinger

$$A_{ij} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{18.2.5}$$

3. *Hyperbolic:* All eigenvalues are nowhere vanishing. One sign differs from the others. Ex: Wave, Klein-Gordon

$$A_{ij} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{18.2.6}$$

18.3 Initial and Boundary Conditions on PDEs in Physics

18.3.1 The Main Idea: Initial Conditions

In physics situations, the classification and types of boundary conditions are typically straightforward: if there are two time derivatives, the equation is hyperbolic and we will need two initial conditions on the entire spatial region to make the solution unique; if there is only a single time derivative, the equation is parabolic and we will need only a single initial condition; if the equation has no time derivatives, the equation is elliptic and the solutions are qualitatively different from the previous two cases. It is easiest to understand the elliptic case from an explicit example.

18.3.2 The Main Idea: Spatial Boundary Conditions

In addition to initial conditions, we will need boundary conditions on the spatial variables. The three main type of boundary conditions encountered in physics are *Dirichlet*, when the value of the solution of the PDE goes to zero on a continuous portion of the boundary, *Neumann*, when the normal (to the boundary) derivative of the solution goes to zero on a continuous portion of the boundary, and *periodic*, when a spatial variable is periodic (for example, on a ring).

The theorems in the optional subsection below, give examples of when a PDE with boundary and initial conditions is guaranteed to have a unique solution. The theorems below consider cases when the (spatial) boundary conditions are either Dirichlet or Neumann on each piecewise smooth piece of the boundary. There are other theorems, not given here, that cover other cases, particularly periodic boundary conditions.

As a mathematical exercise, it would be easy to write down PDEs that do not satisfy a uniqueness theorem. Fortunately, for physicists, the universe provides evidence that unique solutions to the PDEs that are important to physics do exist. So, usually we are not concerned about using the theorems to prove that a solution exists, but rather we are interested in using the theorems to tell us how many of which kinds of boundary and initial conditions we need to specify to ensure that the solution is unique.

18.3.3 Optional Mathematical Details

18.3.3.1 Elliptic Equations

Example: Poisson's Equation

$$\nabla^2 \psi(x_k) = f(x_k) \tag{18.3.1}$$

Theorem: If $\psi(x_k)$ satisfies Poisson's equation throughout a closed, bounded region R and satisfies Dirichlet conditions on the the boundary ∂R of R, then ψ is unique.

Theorem: If $\psi(x_k)$ satisfies Poisson's equation throughout a closed, bounded region R and satisfies Neumann conditions on the the boundary ∂R of R, then ψ is unique up to an additive constant.

Corollary: If the boundary is piecewise smooth, you can specify either Dirichlet or Neumann conditions on each piece. If Dirichlet conditions are satisfied on at least one piece then ψ is unique.

Corollary: If the region R is unbounded (in some or all directions) but $\psi = o(r^{-1/2})$ as $r \to \infty$ (i.e. ψ falls off faster than $r^{-1/2}$) in the unbounded directions, then ψ is unique.

18.3.3.2 Parabolic Equations

Example: Inhomogeneous Diffusion Equation

$$\left(\frac{\partial}{\partial t} - k\nabla^2\right)\psi(t, x_k) = f(x_k) \tag{18.3.2}$$

Theorem: If $\psi(t, x_k)$ satisfies the inhomogeneous diffusion equation throughout a closed, bounded region R and satisfies either Dirichlet *or* Neumann conditions on the the boundary ∂R of R, *and* ψ satisfies the initial condition

$$\psi(t = 0, x_k) = g(x_k) \tag{18.3.3}$$

then ψ is unique.

Corollary: If the spatial boundary is piecewise smooth, you can specify either Dirichlet or Neumann conditions on each piece.

Corollary: If the region R is unbounded (in some or all spatial directions) but $\psi = o(r^{-1/2})$ as $r \to \infty$ (i.e. ψ falls off faster than $r^{-1/2}$) in the unbounded directions, then ψ is unique.

18.3.3.3 Hyperbolic Equations

Example: Inhomogeneous Wave Equation

$$\left(\frac{-1}{v^2}\frac{\partial^2}{\partial t^2} + \nabla^2\right)\psi(t, x_k) = f(x_k) \tag{18.3.4}$$

Theorem: If $\psi(t, x_k)$ satisfies the inhomogeneous wave equation throughout a closed, bounded region R and satisfies either Dirichlet *or* Neumann conditions on the the boundary ∂R of R, *and* ψ satisfies the two initial conditions

$$\psi(t = 0, x_k) = g(x_k) \tag{18.3.5}$$

$$\frac{\partial \psi}{\partial t}(t = 0, x_k) = h(x_k) \tag{18.3.6}$$

then ψ is unique.

Corollary: If the spatial boundary is piecewise smooth, you can specify either Dirichlet or Neumann conditions on each piece.

Corollary: If the region R is unbounded (in some or all spatial directions) but $\psi = o(r^{-1/2})$ as $r \to \infty$ (i.e. ψ falls off faster than $r^{-1/2}$) in the unbounded directions, then ψ is unique.

18.4 Separation of Variables

Definition 18.4.1 Separation of Variables. Separation of variables is a procedure which turns a partial differential equation into a set of ordinary differential equations. ♢

The procedure only works in very special cases involving a high degree of symmetry. Remarkably, the method works for many important physics examples. Furthermore, these examples form important limiting cases that can help with the interpretation of solutions of pde's (typically numerical) that are not obtained by this procedure. Here, we will demonstrate the method on a simple example, the wave equation.

Method. *Step 1:* Write the partial differential equation in appropriate coordinate system. For the wave equation we have:

$$\frac{\partial^2 f}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2 f}{\partial t^2} = 0 \tag{18.4.1}$$

Step 2: Ansatz: ASSUME that the solution $f(x,t)$ can be written as the product of functions, each of which depends on only one variable, in this case x or t, i.e. assume

$$f(x,t) = X(x)T(t) \tag{18.4.2}$$

This is a very strong assumption. Not all solutions will be of this form. However, it turns out that all of the solutions can be written as linear combinations of solutions of this form. The study of when and why this works is called Sturm-Liouville theory.

Plug this assumed solution (18.4.2) into the partial differential equation (18.4.1). Because of the special form for f, the partial derivatives each act on only one of the factors in f.

$$T\frac{d^2 X}{dx^2} - \frac{1}{v^2}X\frac{d^2 T}{dt^2} = 0 \tag{18.4.3}$$

Any partial derivatives that act only on a function of a single variable may be rewritten as total derivatives.

Step 3: Divide by f in the form of (18.4.2). Many, many students forget this step. Don't be one of them! The rest of the procedure doesn't work if you do.

$$\frac{1}{X}\frac{d^2 X}{dx^2} - \frac{1}{v^2}\frac{1}{T}\frac{d^2 T}{dt^2} = 0 \tag{18.4.4}$$

Step 4: Isolate *all* of the dependence on one coordinate on one side of the equation. Do as much algebra as you need to do to achieve this. In our example, notice that in (18.4.4), all of the t dependence is already in one term while all of the dependence on the x variable is in the other term. In this case, the t dependence is trivially isolated by putting the t term on the other side of the equation, without any other algebra on our part.

$$\frac{1}{X}\frac{d^2 X}{dx^2} = \frac{1}{v^2}\frac{1}{T}\frac{d^2 T}{dt^2} \tag{18.4.5}$$

Step 5: Now imagine changing the isolated variable t by a small amount. In principle, the right-hand side of (18.4.5) could change, but nothing on the left-hand side would. (This argument is the magic of the separation of variables procedure–compare it to arguments about constants of the motion from classical mechanics.) Therefore, if the equation is to be true for all values of t, the particular combination of t dependence on the right-hand side must be constant. We will call this constant A. Note that we don't know (yet) whether the constant is positive or negative.

$$\frac{1}{X}\frac{d^2 X}{dx^2} = \frac{1}{v^2}\frac{1}{T}\frac{d^2 T}{dt^2} \equiv A \tag{18.4.6}$$

In this way we have broken our original partial differential equation up into a pair of equations, one of which is an ordinary differential equation involving only t, the other is an ordinary differential equation involving only x.

$$\frac{1}{X}\frac{d^2 X}{dx^2} = A \tag{18.4.7}$$

$$\frac{1}{v^2}\frac{1}{T}\frac{d^2T}{dt^2} = A \tag{18.4.8}$$

The separation constant A appears in both equations.

Step 6: Write each equation in standard form by multiplying each equation by its unknown function to clear it from the denominator.

$$\frac{d^2X}{dx^2} - AX = 0 \tag{18.4.9}$$

$$\frac{d^2T}{dt^2} - Av^2T = 0 \tag{18.4.10}$$

Notice that (18.4.9) is an eigenvalue equation for the operator $\frac{d^2}{dx^2}$. At the moment, the eigenvalue A could be anything. We will use the spatial boundary conditions for a problem that we want to solve to find the possible values of A. Once we have found the possible eigenvalues A, (18.4.10) becomes a second order ordinary differential equation with constant coefficients which you should know how to solve. It is NOT an eigenvalue equation because the value of A is now known. In general, if you are doing the separation of varibles process for n variables, you will get $n-1$ separation constants and therefore $n-1$ eigenvalue equations and an nth ODE which is NOT an eigenvalue equation.

18.5 Separation of Variables for the Hydrogen Atom

We will use the *separation of variables* procedure Section 18.4 on the Schrödinger equation in a central potential. Most of the calculation will involve using this procedure on the Laplacian operator. Since the Laplacian comes up in almost all physics problems with spherical symmetry, you will find yourself using the results of this section many times in your career.

Because there are several spatial dimensions, the procedure requires a number of rounds, each consisting of the same set of six steps. In the first round, we will separate out an ordinary differential equation in the time variable.

Step 1: Write the partial differential equation in appropriate coordinate system. For Schrödinger's equation in any potential we have:

$$H_{\text{op}}\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{18.5.1}$$

Step 2: Assume that the solution Ψ can be written as the product of functions, at least one of which depends on only one variable, in this case t. The other function(s) must not depend at all on this variable, i.e. assume

$$\Psi(r,\theta,\phi,t) = \psi(r,\theta,\phi)T(t) \tag{18.5.2}$$

Plug this assumed solution (18.5.2) into the partial differential equation (18.5.1). Because of the special form for Ψ, the partial derivatives each act on only one of the factors in Ψ:

$$(H_{\text{op}}\psi)\,T = i\hbar\psi\,\frac{dT}{dt} \tag{18.5.3}$$

Any partial derivatives that act only on a function of a single variable may be rewritten as total derivatives.

Step 3: Divide by Ψ in the form of (18.5.2).

$$\frac{1}{\psi}\,(H_{\text{op}}\psi) = i\hbar\frac{dT}{dt}\frac{1}{T} \tag{18.5.4}$$

Step 4: Isolate *all* of the dependence on one coordinate on one side of the equation. Do as much algebra as you need to do to achieve this. In our example, notice that in (18.5.4), all of the t dependence is on the right-hand side of the equation while all of the dependence on the spatial variable is on the other side. In this case, the t dependence is already isolated, without any algebra on our part.

Step 5: Now imagine changing the isolated variable t by a small amount. In principle, the right-hand side of (18.5.4) could change, but nothing on the left-hand side would. Therefore, if the equation is to be true for all values of t, the particular combination of t dependence on the right-hand side must be constant. By convention, we call this constant E.

$$\frac{1}{\psi}\left(H_{\text{op}}\psi\right) = i\hbar\frac{dT}{dt}\frac{1}{T} \stackrel{\text{def}}{=} E \tag{18.5.5}$$

In this way we have broken our original partial differential equation up into a pair of equations, one of which is an ordinary differential equation involving only t, the other is a partial differential equation involving only the three spatial variables:

$$\frac{1}{\psi}H_{\text{op}}\psi = E \tag{18.5.6}$$

$$i\hbar\frac{dT}{dt}\frac{1}{T} = E \tag{18.5.7}$$

The separation constant E appears in both equations.

Step 6: Write each equation in standard form by multiplying each equation by its unknown function to clear it from the denominator:

$$H_{\text{op}}\psi = E\psi \tag{18.5.8}$$

$$\frac{dT}{dt} = -\frac{i}{\hbar}ET \tag{18.5.9}$$

Notice that (18.5.8) is an eigenvalue equation for the operator H_{op}. You may never have thought of the derivation of this "time independent version of the Schrödinger equation" from the Schrödinger equation as just a simple example of the separation of variables procedure. At the moment, the eigenvalue E could be anything. Much of the rest of the Paradigm will be directed toward finding the possible values of E!

Now we must repeat the steps until each of the variables has been separated out into its own ordinary differential equation. In the next round, we will isolate the r dependence.

Step 1: Since we want to isolate the r dependence, we must rewrite H_{op} to show the r dependence explicitly using (24.3.8):

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}L^2_{\text{op}}\right]\psi + U(r)\psi = E\psi \tag{18.5.10}$$

Step 2: Assume $\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$.

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)Y - \frac{1}{\hbar^2 r^2}R(L^2_{\text{op}}Y)\right] + U(r)RY = ERY \tag{18.5.11}$$

Step 3:

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{d}{dr}\frac{1}{R}\left(r^2\frac{dR}{dr}\right) - \frac{1}{\hbar^2 r^2}\frac{1}{Y}(L^2_{\text{op}}Y)\right] + U(r) = E \tag{18.5.12}$$

Step 4: To isolate the r dependence we must first clear the r dependence from the angular term (involving angular derivatives in $L_{\rm op}$ and angular functions in Y). To do this, we need to multiply (18.5.12) by r^2 to clear this factor out of the denominators of the angular pieces. Further rearranging (18.5.12) to get all of the r dependence on the right-hand side, we obtain:

$$-\frac{1}{\hbar^2}\frac{1}{Y}(L^2_{\rm op}Y) = -\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\frac{1}{R} - \frac{2\mu}{\hbar^2}\big(E-U(r)\big)r^2 \tag{18.5.13}$$

Step 5: In this case, I have called the separation constant A.

$$-\frac{1}{\hbar^2}\frac{1}{Y}(L^2_{\rm op}Y) = -\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\frac{1}{R} - \frac{2\mu}{\hbar^2}\big(E-U(r)\big)r^2 \stackrel{\rm def}{=} A \tag{18.5.14}$$

In principle, A can be any complex number.

Step 6: Rearranging (18.5.14) slightly, we obtain the radial and angular equations in the more standard form:

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu}{\hbar^2}\big(E-U(r)\big)r^2\,R + AR = 0 \tag{18.5.15}$$

$$L^2_{\rm op}Y + \hbar^2 AY = 0 \tag{18.5.16}$$

Notice that the only place that the central potential enters the set of differential equations is in the radial equation (18.5.15). (18.5.15) is not yet in the form of an eigenvalue equation since it contains two unknown constants E and A. (18.5.16) is an eigenvalue equation for the operator $L^2_{\rm op}$ with eigenvalue $\hbar^2 A$; it is independent of the form of the central potential.

In the last round, we must separate the θ dependence from the ϕ dependence. I will leave this as an important Practice Problem. The answer is:

$$\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) - A\sin^2\theta P - BP = 0 \tag{18.5.17}$$

$$\frac{d^2\Phi}{d\phi^2} + B\Phi = 0 \tag{18.5.18}$$

is an eigenvalue equation for the operator $d^2/d\phi^2$ with eigenvalue B. is not yet in the form of an eigenvalue equation since it contains two unknown constants A and B.

We started with a partial differential equation in four variables and we ended up with four ordinary differential equations (18.5.9), (18.5.15), (18.5.17), (18.5.18) by introducing *three* separation constants (E, A, and B). You should always get one fewer separation constant than the number of variables you started with; each separation constant should appear in two of the final set of equations.

Chapter 19

Eigen Expansions

19.1 Sturm–Liouville Theory

The Main Idea. When you use the separation of variables procedure on a PDE, you end up with one or more ODEs that are eigenvalue problems, i.e. they contain an unknown constant that comes from the separation constants.

These ODEs are called Sturm-Liouville equations. By solving the ODEs for particular boundary conditions, we find particular allowed values for the eigenvalues. The essence of the theorems below is that the solutions of the ODEs for these special boundary conditions and eigenvalues form an orthogonal set. These solutions can be used to form a basis of solutions of the original PDE. The rest of this section states the technical mathematics theorems for the most important cases where this process works. If you enjoy mathematics, please read on. If not, then rest assured that the mathematics guarantees that the separation of variables process will work whenever you are asked to use it in undergraduate physics.

19.1.1 Optional Mathematical Details

Sturm-Liouville Theory for Boundary-Value Problems. A second order Sturm–Liouville problem is a homogeneous boundary value problem of the form

$$[P(x)\,y']' + Q(x)\,y + \lambda\,w(x)\,y = 0 \tag{19.1.1}$$

$$\alpha_1\,y(a) + \beta_1\,y'(a) = 0 \tag{19.1.2}$$

$$\alpha_2\,y(b) + \beta_2\,y'(b) = 0 \tag{19.1.3}$$

where P, P', Q, w are continuous and real on $[a, b]$, and P and w are positive.

Theorem: For y_1 and y_2 two linearly independent solutions of the homogeneous differential equation, *nontrivial* solutions of the homogeneous boundary value problem exist iff

$$\begin{vmatrix} \alpha_1\,y_1(a) + \beta_1\,y_1'(a) & \alpha_1\,y_2(a) + \beta_1\,y_2'(a) \\ \alpha_2\,y_1(b) + \beta_2\,y_1'(b) & \alpha_2\,y_2(b) + \beta_2\,y_2'(b) \end{vmatrix} = 0 \tag{19.1.4}$$

Definition: Values of λ for which nontrivial solutions exist are called eigenvalues. The corresponding solutions are called eigenfunctions.

Theorem: The eigenvalues of a homogeneous Sturm-Liouville problem are real and non-negative and can be arranged in a strictly increasing infinite sequence

$$0 \le \lambda_1 < \lambda_2 < \lambda_3 < \dots \tag{19.1.5}$$

and $\lambda_n \to \infty$ as $n \to \infty$.

Theorem: For each eigenvalue, there exists exactly one linearly independent eigenfunction, y_n. These eigenfunctions for differing eigenvalues are orthogonal with respect to the inner product:

$$(y_n, y_m)_w = \int_a^b y_n(x)\, y_m(x)\, w(x)\, dx = N_n \delta_{n,m} \tag{19.1.6}$$

Theorem: The eigenfunctions y_n span the vector space of piecewise smooth functions satisfying the boundary conditions of the Sturm-Liouville problem. (Convergence in the mean, not pointwise.)

$$f(x) = \sum_{n=1}^{\infty} c_n\, y_n(x) \tag{19.1.7}$$

where the c_n's are given by:

$$c_n = \frac{1}{N_n}(y_n, f)_w = \frac{1}{N_n} \int_a^b y_n^*(x)\, f(x)\, w(x)\, dx \tag{19.1.8}$$

Sturm-Liouville Theory for Periodic Systems. A second order periodic Sturm–Liouville problem is a homogeneous problem of the form

$$[P(x)\, y']' + Q(x)\, y + \lambda\, w(x)\, y = 0 \tag{19.1.9}$$

where P, P', Q, w are continuous and real on $[a, b]$, and P and w are positive, and

$$\left[P(x)\left(f^*(x)\, g'(x) - f^{*\prime}(x)\, g(x)\right)\right]\Big|_a^b = 0 \tag{19.1.10}$$

for $f(x)$ and $g(x)$ and two vectors in the vector space.

Definition: Values of λ for which nontrivial solutions of the periodic Sturm-Liouville problem exist are called eigenvalues. The corresponding solutions are called eigenfunctions.

Theorem: The eigenvalues of a periodic Sturm-Liouville problem are real.

Theorem: For each eigenvalue, there exist linearly independent eigenfunctions, y_n. These eigenfunctions for differing eigenvalues are orthogonal with respect to the inner product:

$$(y_n, y_m)_w = \int_a^b y_n(x)\, y_m(x)\, w(x)\, dx = N_n \delta_{n,m} \tag{19.1.11}$$

Eigenfunctions with the same eigenvalue can be orthogonalized using Gram-Schmidt orthogonalization.

Theorem: The eigenfunctions y_n span the vector space of piecewise smooth functions satisfying the boundary conditions of the Sturm-Liouville problem. (Convergence in the mean, not pointwise.)

$$f(x) = \sum_{n=1}^{\infty} c_n\, y_n(x) \tag{19.1.12}$$

where the c_n's are given by:

$$c_n = \frac{1}{N_n}(y_n, f)_w = \frac{1}{N_n} \int_a^b y_n^*(x)\, f(x)\, w(x)\, dx \tag{19.1.13}$$

19.2 Legendre Polynomials

Legendre polynomials can be found from **Rodrigues' formula**

$$P_\ell(z) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dz^\ell} \left(z^2 - 1\right)^\ell \tag{19.2.1}$$

Rodrigues' Formula can be used to generate the polynomials quickly. To do this, write

$$\left(z^2 - 1\right)^\ell = (z-1)^\ell (z+1)^\ell = a^\ell b^\ell \tag{19.2.2}$$

and use the product rule

$$\begin{aligned} \frac{d^\ell}{dz^\ell} \left(z^2 - 1\right)^\ell = &\left(\frac{d^\ell a}{dz^\ell}\right) b + \ell \left(\frac{d^{\ell-1} a}{dz^{\ell-1}}\right) \left(\frac{db}{dz}\right) \\ &+ \frac{\ell(\ell-1)}{2!} \left(\frac{d^{\ell-2} a}{dz^{\ell-2}}\right) \left(\frac{d^2 b}{dz^2}\right) + \ldots + a \left(\frac{d^\ell b}{dz^\ell}\right) \end{aligned} \tag{19.2.3}$$

where the coefficients in the i^{th} term in the product is the **binomial coefficient**

$$\binom{\ell}{i} = \binom{\ell}{\ell - i} = \frac{\ell!}{(\ell - i)!\, i!} \tag{19.2.4}$$

The first few Legendre polynomials are:

$$P_0(z) = 1 \tag{19.2.5}$$
$$P_1(z) = z \tag{19.2.6}$$
$$P_2(z) = \frac{1}{2}\left(3z^2 - 1\right) \tag{19.2.7}$$
$$P_3(z) = \frac{1}{2}\left(5z^3 - 3z\right) \tag{19.2.8}$$
$$P_4(z) = \frac{1}{8}\left(35z^4 - 30z^2 + 3\right) \tag{19.2.9}$$
$$P_5(z) = \frac{1}{8}\left(63z^5 - 70z^3 + 15z\right) \tag{19.2.10}$$

There are several useful patterns to the Legendre polynomials:

- $P_\ell(z)$ is a polynomial of degree ℓ.
- Each $P_\ell(z)$ contains only odd or only even powers of z, depending on whether ℓ is even or odd. Therefore, each $P_\ell(z)$ is either an even or an odd function.
- The overall coefficient for each solution is conventionally chosen so that $P_\ell(1) = 1$. *As discussed in Section 19.3, this is an inconvenient convention that we are stuck with!*
- Since the differential operator in (16.2.1) is Hermitian (unproven), we are guaranteed by a deep theorem of mathematics (Sturm-Liouville theory, see Section 19.1) that the Legendre polynomials are orthogonal for different values of ℓ (just as with Fourier series)

  The orthogonality and normalization properties of the Legendre polynomials can be found by using Rodrigues' Formula and repeated integration by parts, noting that the "surface terms" always vanish.

i.e.

$$\int_{-1}^{1} P_k^*(z)\, P_\ell(z)\, dz = \frac{\delta_{k\ell}}{\ell + \frac{1}{2}} \tag{19.2.11}$$

The "squared norm" of P_ℓ is just $1/(\ell + \frac{1}{2})$. To normalize each $P_\ell(z)$, it should be multiplied by $\sqrt{\ell + \frac{1}{2}}$.

Notice that **Legendre's equation**, i.e. the differential equation

$$\frac{\partial^2 P}{\partial z^2} - \frac{2z}{1-z^2}\frac{\partial P}{\partial z} + \frac{\ell(\ell+1)}{1-z^2} P = 0 \tag{19.2.12}$$

is a *different* equation for different values of ℓ. For a given value of ℓ, you should expect two solutions of (19.2.12). We have only given one, for the special case $\ell \in \{0, 1, 2, 3, \dots\}$. It turns out that the *other* solution for these values of ℓ and both solutions for other values ℓ are not regular (i.e. blow up) at $z = \pm 1$. We can often discard these irregular solutions as unphysical for the problems we are solving.

19.3 Legendre Polynomial Series

There is a very powerful mathematical theorem which says that *any* sufficiently smooth function $f(z)$, defined on the interval $-1 < z < 1$, can be expanded as a linear combination of Legendre polynomials

$$f(z) = \sum_{\ell=0}^{\infty} c_\ell\, P_\ell(z) \tag{19.3.1}$$

(This theorem is the analogue of the theorem which says that any sufficiently smooth periodic function can be expanded in a Fourier series.) You will have several occasions in physics to expand functions in Legendre polynomial series, so we will explore the technique in this section.

We can find the coefficients c_ℓ by taking the inner product of both sides of (19.3.1) in turn with each "basis vector" P_ℓ and using (19.2.11). This yields

$$\begin{aligned}
\int_{-1}^{1} P_k^*(z)\, f(z)\, dz &= \int_{-1}^{1} P_k^*(z) \sum_{\ell=0}^{\infty} c_\ell\, P_\ell(z)\, dz \\
&= \sum_{\ell=0}^{\infty} c_\ell \int_{-1}^{1} P_k^*(z)\, P_\ell(z)\, dz \\
&= \sum_{\ell=0}^{\infty} c_\ell \frac{\delta_{k\ell}}{\ell + \frac{1}{2}} \\
&= \frac{c_k}{k + \frac{1}{2}}
\end{aligned} \tag{19.3.2}$$

or equivalently

$$c_k = \left(k + \frac{1}{2}\right) \int_{-1}^{1} P_k^*(z)\, f(z)\, dz \tag{19.3.3}$$

This expression should be compared with the exponential version of a Fourier series for $f(z)$ on the same interval $-1 \le z \le 1$, namely

$$f(z) = \sum_{n=-\infty}^{\infty} C_n \, e^{in\pi z} \tag{19.3.4}$$

where

$$C_n = \frac{1}{2} \int_{-1}^{1} e^{-in\pi z} f(z) \, dz \tag{19.3.5}$$

Note the analogous role played by the *normalization constants* $k + \frac{1}{2}$ and $\frac{1}{2}$. If we had made an unconventional, but more convenient, choice for the normalization for the Legendre polynomials such that the value of the integrals in (19.2.11) were simply $\delta_{k\ell}$, then we would not need to carry around the extra factor of $k + \frac{1}{2}$ in (19.3.3).

Example 19.3.1 Example: Legendre Expansion of $\varepsilon(z)$. Consider the step function

$$\varepsilon(z) = 2\,\Theta(z) - 1 = \begin{cases} +1 & (z > 0) \\ -1 & (z < 0) \end{cases} \tag{19.3.6}$$

where Θ is the Heaviside step function; note that $\varepsilon(z)$ is an *odd* function of z. Using (19.3.3) leads to

$$\begin{aligned} c_\ell &= \left(\ell + \frac{1}{2}\right) \int_{-1}^{1} P_\ell^*(z) \, \varepsilon(z) \, dz \\ &= -\left(\ell + \frac{1}{2}\right) \int_{-1}^{0} P_\ell^*(z) \, dz + \left(\ell + \frac{1}{2}\right) \int_{0}^{1} P_\ell^*(z) \, dz \end{aligned} \tag{19.3.7}$$

and each integral in the final expression is an elementary integral of a polynomial. Furthermore, it is easily seen that these two integrals cancel if ℓ is even, and add if ℓ is odd, so that

$$c_\ell = \begin{cases} 0 & (\ell \text{ even}) \\ 2\left(\ell + \frac{1}{2}\right) \int_{0}^{1} P_\ell^*(z) \, dz & (\ell \text{ odd}) \end{cases} \tag{19.3.8}$$

These coefficients are easily evaluated on Maple for as many values of ℓ as desired. □

19.4 Legendre Expansions

Legendre functions have many remarkable properties.

Figure 19.4.1 below shows the mth order Legendre expansion of a given function.

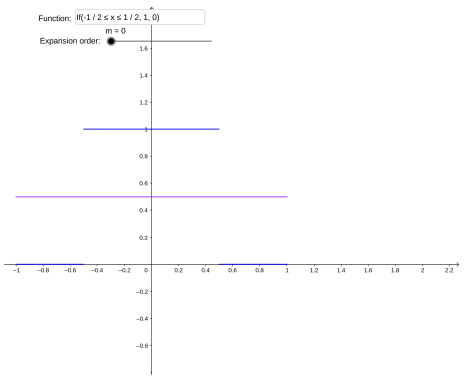


Figure 19.4.1 The mth order Legendre expansion of a given function.

Figure 19.4.2 below allows you to see the effect of varying the Legendre coefficients individually while trying to guess the Legendre expansion of a given function, using *unnormalized* Legendre polynomials.

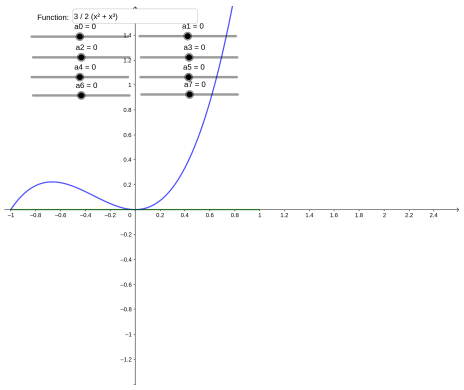


Figure 19.4.2 Varying the individual Legendre coefficients, using unnormalized Legendre polynomials.

Figure 19.4.3 below allows you to see the effect of varying the Legendre coefficients individually while trying to guess the Legendre expansion of a given function, using *normalized* Legendre polynomials. [1]

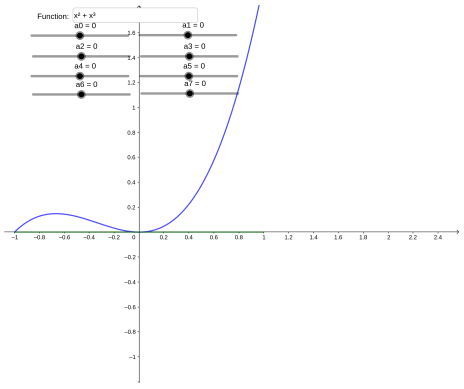


Figure 19.4.3 Varying the individual Legendre coefficients, using normalized Legendre polynomials.

[1] Since the normalization involves square roots, the discrete coefficients allowed in Figure 19.4.3 are not sufficient to exactly match the given function. How close can you get?

19.5 Legendre Series: Worked Example

You are encouraged to explore the Legendre basis functions using the applet in Figure 19.4.1 before working through the example here.

The *unrenormalized* Legendre polynomials can be defined as

$$P_0(x) = 1, \tag{19.5.1}$$
$$P_1(x) = x, \tag{19.5.2}$$
$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x) \tag{19.5.3}$$

and satisfy the orthogonality condition

$$\int_{-1}^{1} P_m(x)P_n(x) = \frac{2}{2n+1}\delta_{mn}. \tag{19.5.4}$$

We can expand any function $f(x)$ on the interval $-1 \leq x \leq 1$ in terms of these Legendre polynomials as

$$f(x) = \sum_{0}^{\infty} a_m P_m(x) \tag{19.5.5}$$

and use (19.5.4) to determine the coefficients as

$$a_n = \frac{2n+1}{2}\int_{-1}^{1} f(x)P_n(x). \tag{19.5.6}$$

You can use the Sage code below to display the Legendre polynomial $P_n(x)$ for any integer value of n, and then its graph.

```
pretty_print_default(True)
n=2
legendre_P(n,x)
```

```
plot(legendre_P(n,x),x,-1,1)
```

Now we will use the integral expressions (19.5.6) for the coefficients in a Legendre expansion to work out an example, the Legendre series for the function $f(x) = \frac{3}{2}(x^2 + x^3)$. Then you will plot the individual terms in the Legendre series and their partial sums using an applet.

You can use the Sage code below to calculate the value of the integral for the first coefficient, a_0.

```
m=0
f=3/2*(x^2+x^3)
(2*m+1)/2*integrate(f*legendre_P(m,x),x,-1,1)
```

Using the applet in Figure 19.5.1, set the a_0 slider to correspond to the value you just calcuated. [1] Compare your approximate Legendre series, containing just one term (shown in green), to the actual function (shown in blue).

[1] You can use the right and left arrow keys to move the selected slider in increments of 0.5; holding down the shift key as well changes the increment to 0.05.

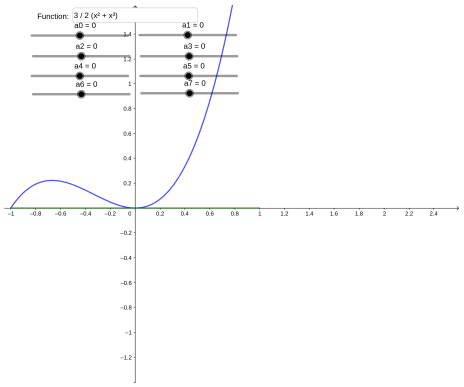


Figure 19.5.1 Varying the individual Legendre coefficients, using unnormalized Legendre polynomials.

Now you can alter the Sage code above to compute the other coefficients. After each calculation, move the corresponding slider to the value you obtain, and compare the approximation to the given function.

If you move the sliders one by one, resetting the others to zero, you will see how much each individual term contributes to the Legendre series.

If you don't reset the other sliders, but instead combine the contributions from each slider, the applet plots the sum of the corresponding terms (in green), representing an approximation to the actual function (in blue). In the given example, you should obtain an exact match when you include all of the terms with $m = 0, 1, 2, 3$. In general, there are an infinite number of nonzero terms in the Legendre series; your approximation will get better and better as you include more terms.

19.6 Associated Legendre Functions

We now return to (24.11.6) to consider the cases with $m \neq 0$. We can solve these equations with (a slightly more sophisticated version of) the series techniques from the $m = 0$ case. We would again find solutions that are regular at $z = \pm 1$ whenever we choose $A = -\ell(\ell+1)$ for $\ell \in \{0, 1, 2, 3, ...\}$. With this value for A, we obtain the standard form of Legendre's associated equation, namely

$$\left(\frac{\partial^2}{\partial z^2} - \frac{2z}{1-z^2} \frac{\partial}{\partial z} - \frac{m^2}{(1-z^2)^2} + \frac{\ell(\ell+1)}{1-z^2} \right) P(z) = 0 \tag{19.6.1}$$

Recall that this equation was obtained by separating variables in spherical coordinates. Solutions of this equation which are regular at $z = \pm 1$ are called *associated Legendre functions*, and turn out to be given by

$$\begin{aligned} P_\ell^{-m}(z) = P_\ell^m(z) &= (1-z^2)^{m/2} \frac{d^m}{dz^m} \left(P_\ell(z) \right) \\ &= (1-z^2)^{m/2} \frac{d^{m+\ell}}{dz^{m+\ell}} \left((z^2-1)^\ell \right) \end{aligned} \tag{19.6.2}$$

where $m \geq 0$. [1] Note that if $z = \cos\theta$, then $P_\ell(z)$ is a polynomial in $\cos\theta$, while

$$(1-z^2)^{m/2} = (\sin^2\theta)^{m/2} = \sin^m\theta \tag{19.6.3}$$

so that $P_\ell^m(z)$ is a polynomial in $\cos\theta$ times a factor of $\sin^m\theta$. Some other properties of the associated Legendre functions are

[1] Some authors define $P_\ell^{-m}(z)$ differently.

- $P_\ell^m(z) = 0$ if $m > \ell$
- $P_\ell^{-m}(z) = P_\ell^m(z)$
- $P_\ell^m(\pm 1) = 0$ for $m \neq 0$ (cf. factor of $(1-z^2)^{m/2}$)
- $P_\ell^m(-z) = (-1)^{\ell_m} P_\ell^m(z)$ (behavior under parity)
- $\displaystyle\int_{-1}^{1} P_\ell^m(z) P_q^m(z)\, dz = \frac{2}{(2\ell+1)} \frac{(\ell+m)!}{(\ell-m)!}\, \delta_{\ell q}$

The last property shows that for each given value of m, the Associated Legendre functions form an orthonormal basis on the interval $-1 \leq z \leq 1$. Any function on this interval can be expanded in terms of anyone of these bases.

19.7 Spherical Harmonics

We have found that normalized solutions of the ϕ equation (18.5.18) satisfying periodic boundary conditions are

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}}\, e^{im\phi} \qquad (m = 0, \pm 1, \pm 2, ...) \tag{19.7.1}$$

and normalized solutions of the θ equation (18.5.17) which are regular at the poles are given by

$$P(\cos\theta) = \sqrt{\frac{(2\ell+1)}{2} \frac{(\ell-|m|)!}{(\ell+|m|)!}}\, P_\ell^m(\cos\theta) \tag{19.7.2}$$

Combining these yields via multiplication (we assumed solutions of this type when we first did the separation of variables procedure), we obtain the *spherical harmonics*

$$Y_\ell^m(\theta,\phi) = (-1)^{(m+|m|)/2} \sqrt{\frac{(2\ell+1)}{4\pi} \frac{(\ell-|m|)!}{(\ell+|m|)!}}\, P_\ell^m(\cos\theta)\, e^{im\phi} \tag{19.7.3}$$

where the somewhat peculiar choice of phase is conventional.

The spherical harmonics are orthonormal on the unit sphere:

$$\int_0^{2\pi} \int_0^{\pi} \left(Y_{\ell_1}^{m_1}\right)^* Y_{\ell_2}^{m_2} \sin\theta\, d\theta\, d\phi = \delta_{\ell_1 \ell_2} \delta_{m_1 m_2} \tag{19.7.4}$$

since $dz = \sin\theta\, d\theta$. They are complete in the sense that any sufficiently smooth function f on the unit sphere can be expanded in a *Laplace series* as

$$f(\theta,\phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m}\, Y_\ell^m(\theta,\phi) \tag{19.7.5}$$

where

$$a_{\ell m} = \int_0^{2\pi} \int_0^{\pi} \left(Y_\ell^m\right)^* f(\theta,\phi)\, \sin\theta\, d\theta\, d\phi \tag{19.7.6}$$

Example 19.7.1 **Example.** Suppose you want a function of (θ,ϕ) which

satisfies

$$f(\theta,\phi) = \begin{cases} \sin\theta & 0 < \theta < \frac{\pi}{2} \\ 0 & \text{otherwise} \end{cases} \tag{19.7.7}$$

Then f takes the form (19.7.5), and the constants $a_{\ell m}$ can be determined from (19.7.6), yielding

$$\begin{aligned} a_{\ell m} &= \int_0^{2\pi}\int_0^{\pi/2} (Y_\ell^m)^* \sin^2\theta \, d\theta \, d\phi \\ &= N_{\ell m} \int_0^{2\pi} e^{-im\phi}\, d\phi \int_0^{\pi/2} P_\ell^m(\cos\theta)\, \sin^2\theta \, d\theta \end{aligned} \tag{19.7.8}$$

where

$$N_{\ell m} = (-1)^{(m+|m|)/2} \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}} \tag{19.7.9}$$

Thus,

$$a_{\ell m} = \begin{cases} 0 & (m \neq 0) \\ \sqrt{(2\ell+1)\,\pi} \displaystyle\int_0^{\pi/2} P_\ell(\cos\theta)\, \sin^2\theta \, d\theta & (m = 0) \end{cases}$$

For $m = 0$, the integral is most easily computed with the substitution $z = \cos\theta$; the first few coefficients are:

$$\begin{aligned} a_{00} &= \frac{\pi}{8} \qquad a_{10} = \frac{1}{2} \qquad a_{20} = -\frac{5\pi}{64} \\ a_{30} &= -\frac{7}{12} \qquad a_{40} = -\frac{9\pi}{512} \qquad a_{50} = \frac{77}{240} \end{aligned} \tag{19.7.10}$$

(each of which should be multiplied by $\sqrt{4\pi/(2\ell+1)}$). As you can check by graphing, however, it requires at least twice this many terms to obtain a good approximation. □

19.8 Visualizing Spherical Harmonics

The spherical harmonics

$$Y_\ell{}^m(\theta,\phi) = N e^{im\phi} P_\ell{}^m(\cos\theta)$$

with ℓ a nonnegative integer and m an integer satisfying $|m| \leq \ell$ are solutions of the partial differential equation

$$r^2\nabla^2 Y_\ell{}^m = -\ell(\ell+1) Y_\ell{}^m$$

where $P_\ell{}^m$ is an associated Legendre polynomial, and ∇^2 is the Laplacian on the sphere, that is

$$\nabla^2 f = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2}$$

and N is a normalization factor.

You can print the first few spherical harmonics using the following Sage code.

```
pretty_print_default(True)
theta,phi=var('theta,phi')
@interact
def _(l=(0,5,1)):
    @interact
    def _(m=slider(-l,l,step_size=1,default=0)):
        spherical_harmonic(l,m,theta,phi).show()
```

You can also explore the graphs of the spherical harmonics using Sage. The code below plots the squared magnitude (probability density) $|Y_\ell{}^m|^2$ of the first few spherical harmonics in three ways: using color on the unit sphere, as the distance from the origin, and as the distance from the unit sphere.

```
cm=colormaps.hsv
theta,phi=var('theta,phi')
@interact
def _(l=slider(0,5,step_size=1)):
    @interact
    def _(m=slider(-l,l,default=0,step_size=1)):
        sh=spherical_harmonic(l,m,theta,phi)
        max2=max(flatten([[abs(spherical_harmonic(l,m,theta,phi))^2
                           for phi in [2*p*pi/10 for p in
                               range(1)]]
                          for theta in [q*pi/10 for q in
                              range(11)]]))
        max2a=max(flatten([[1+abs(spherical_harmonic(l,m,theta,phi))^2
                           for phi in [2*p*pi/10 for p in
                               range(1)]]
                          for theta in [q*pi/10 for q in
                              range(11)]]))
        def col(phi,theta):
            return
                float(abs(spherical_harmonic(l,m,theta,phi))^2/max2)
        sph1=spherical_plot3d(1,(phi,0,2*pi),(theta,0,pi),
                              plot_points=50,frame=False,color=(col,cm))
        shp2=spherical_plot3d(abs(sh)^2/max2,(phi,0,2*pi),(theta,0,pi),
                              plot_points=50,frame=False,color=(col,cm))
        shp3=spherical_plot3d(1+abs(sh)^2/max2a,(phi,0,2*pi),(theta,0,pi),
                              plot_points=50,frame=False,color=(col,cm))
        shp=sph1.translate((2,-2,0))+shp2+shp3.translate((-2,2,0))
        show(shp)
```

Here are the (magnitudes of the) real and imaginary parts of the spherical harmonics, along with the overall magnitude.

```
cm=colormaps.hsv
theta,phi=var('theta,phi')
@interact
def _(l=slider(0,5,step_size=1)):
    @interact
    def _(m=slider(-l,l,default=0,step_size=1)):
        sh=spherical_harmonic(l,m,theta,phi)
        mr=max(flatten([[abs(real(spherical_harmonic(l,m,theta,phi)))
                           for phi in [2*p*pi/10 for p in
                               range(11)]]
                          for theta in [q*pi/10 for q in
```

```
                            range(11)]]))
        mi=max(flatten([[abs(imag(spherical_harmonic(l,m,theta,phi)))
                         for phi in [2*p*pi/10 for p in
                             range(11)]]
                        for theta in [q*pi/10 for q in
                            range(11)]]))
        mx=max(flatten([[abs(spherical_harmonic(l,m,theta,phi))
                         for phi in [2*p*pi/10 for p in
                             range(11)]]
                        for theta in [q*pi/10 for q in
                            range(11)]]))
        if mi==0:
            mi=1
        def col(phi,theta):
            return
                float(abs(spherical_harmonic(l,m,theta,phi))/mx)
        sphr=spherical_plot3d(abs(real(sh))/mr,(phi,0,2*pi),(theta,0,pi),
                              plot_points=50,frame=False,color=(col,cm))
        shpi=spherical_plot3d(abs(imag(sh))/mi,(phi,0,2*pi),(theta,0,pi),
                              plot_points=50,frame=False,color=(col,cm))
        shpa=spherical_plot3d(abs(sh)/mx,(phi,0,2*pi),(theta,0,pi),
                              plot_points=50,frame=False,color=(col,cm))
        shp=sphr.translate((2,-2,0))+shpi+shpa.translate((-2,2,0))
        show(shp)
```

Here are the signed values of the real and imaginary parts of the spherical harmonics, along with the overall magnitude. (The sign is indicated by color only, not by allowing the radius to become negative.)

```
cm=colormaps.hsv
theta,phi=var('theta,phi')
@interact
def _(l=slider(0,5,step_size=1)):
    @interact
    def _(m=slider(-l,l,default=0,step_size=1)):
        sh=spherical_harmonic(l,m,theta,phi)
        mr=max(flatten([[abs(real(spherical_harmonic(l,m,theta,phi)))
                         for phi in [2*p*pi/10 for p in
                             range(11)]]
                        for theta in [q*pi/10 for q in
                            range(11)]]))
        mi=max(flatten([[abs(imag(spherical_harmonic(l,m,theta,phi)))
                         for phi in [2*p*pi/10 for p in
                             range(11)]]
                        for theta in [q*pi/10 for q in
                            range(11)]]))
        mx=max(flatten([[abs(spherical_harmonic(l,m,theta,phi))
                         for phi in [2*p*pi/10 for p in
                             range(11)]]
                        for theta in [q*pi/10 for q in
                            range(11)]]))
        if mi==0:
            mi=1
        def colr(phi,theta):
            return
                float(1/2+real(spherical_harmonic(l,m,theta,phi))/mx/2)
        def coli(phi,theta):
```

```
            return
                float(1/2+imag(spherical_harmonic(l,m,theta,phi))/mx/2)
        def cola(phi,theta):
            return
                float(1/2+abs(spherical_harmonic(l,m,theta,phi))/mx/2)
        sphr=spherical_plot3d(abs(real(sh))/mr,(phi,0,2*pi),(theta,0,pi),
                              plot_points=50,frame=False,color=(colr,cm))
        shpi=spherical_plot3d(abs(imag(sh))/mi,(phi,0,2*pi),(theta,0,pi),
                              plot_points=50,frame=False,color=(coli,cm))
        shpa=spherical_plot3d(abs(sh)/mx,(phi,0,2*pi),(theta,0,pi),
                              plot_points=50,frame=False,color=(cola,cm))
        shp=sphr.translate((2,-2,0))+shpi+shpa.translate((-2,2,0))
        show(shp)
```

Finally, here you can graph (using color only) the squared magnitude of an arbitrary (complex!) linear combination of spherical harmonics, each entered as "$Y(\ell, m)$". (Use I for i, and submit your combination by pressing Enter.)

```
cm=colormaps.hsv
l,m,theta,phi=var('l,m,theta,phi')
Y(l,m)=spherical_harmonic(l,m,theta,phi)
@interact
def _(YY=input_box(0,label="Sum␣=")):
    def YYe(T,P):
        return YY.subs(phi==P).subs(theta==T)
    maxx=max(flatten([[abs(YYe(q*pi/10,2*p*pi/10))^2
                       for p in range(11)] for q in
                           range(11)]))
    if maxx==0:
        maxx=1
    def col(P,T):
        return float(abs(YYe(T,P))^2/maxx)
    YYg=spherical_plot3d(1,(phi,0,2*pi),(theta,0,pi),
                         plot_points=50,frame=False,color=(col,cm))
    show(YYg)
```

Chapter 20

Fourier Series

20.1 Fourier Series Motivation

UNDER DEVELOPMENT--Add the example of the Fourier series for a pendulum that is NOT in the small angle approximation. Change the figure below.

If a room full of students is asked to sketch an example of a periodic function, at least half will draw a sine or cosine. This is a great choice in the sense that sines and cosines are particularly simple and easy to deal with algebraically. (Even easier are complex exponentials – more about this later.) However, there are many other periodic functions that are not so simple. These functions can represent oscillatory phenomena that occur in many places in nature. Fortunately for us, it turns out that we can express *all* periodic phenomena as (possibly infinite) sums of sines and cosines. These sums are called Fourier Series.

Fourier Series are often used to approximate a function by giving the first few terms. In Figure 20.1.1 you can see how well the first few terms (shown in purple) approximate a periodic step function (shown in blue), with period $L = 1$. You can also use this applet to approximate another function of your choice by entering it in the box labeled "Function". (The applet will automatically convert your function into a periodic function with period 1.)

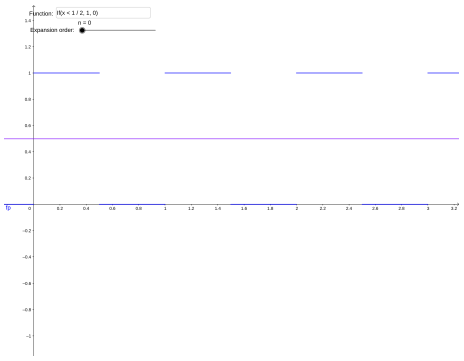


Figure 20.1.1 The first few partial sums in the Fourier series for a step function. Move the slider to increase the number of terms in the sum.

20.2 Fourier Series Overview

The basic idea of a Fourier series is that any (piecewise smooth) periodic function can be accurately represented by a (possibly infinite) sum of sine and cosine functions whose period is an integer multiple of the period of the function. The formula for the Fourier series for the $f(\theta)$ with period 2π (i.e. $f(\theta + 2\pi) = f(\theta)$) is

$$f(\theta) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos n\theta + \sum_{n=1}^{\infty} b_n \sin n\theta \tag{20.2.1}$$

The extra factor of $\frac{1}{2}$ in the a_0 term is a convention. Note, there is no b_0 term since $\sin 0$ is identically zero.

The coefficients a_n and b_n are uniquely determined by $f(\theta)$. The formulas are

$$a_n = \frac{1}{\pi}\int_0^{2\pi} \cos(nx)\, f(x)\, dx$$
$$b_n = \frac{1}{\pi}\int_0^{2\pi} \sin(nx)\, f(x)\, dx$$

The derivation of the coefficients for a given $f(\theta)$ can be found in Section 20.4. The derivation is straightforward and completely analogous to finding coefficients for vectors that are arrows in space. It is also analogous to many such calculations that you will do with other, more abstract vector spaces, so it is well worth your time to work through. The geometric idea behind the formulas for the coefficients can be found in Section 14.5, Section 14.6, an Section 14.7.

In applied settings, you will want formulas for Fourier series involving variables with dimensions. Alternative versions can be found in Section 20.5. Most often, a finite number of terms in the Fourier series are used to approximate a periodic function. You can explore how this works in Section 20.7, Section 20.8, an Section 20.10. In cases with high symmetry, you may be able to simplify your calculations by exploiting the symmetries of the harmonic functions, see Section 20.11.

20.3 Fourier Basis Functions

Before we jump into the details of Fourier series, use the applet below to remind yourself of how the graphs of $\sin(mx)$ and $\cos(mx)$ depend on the parameter m.

Activity 20.3.1 Visualizing the Fourier Basis Functions. Use the applet below to explore the basis functions. One at a time, set each slider to 1, look at the resulting function, and return that slider to 0. Make a note of any patterns that you see.

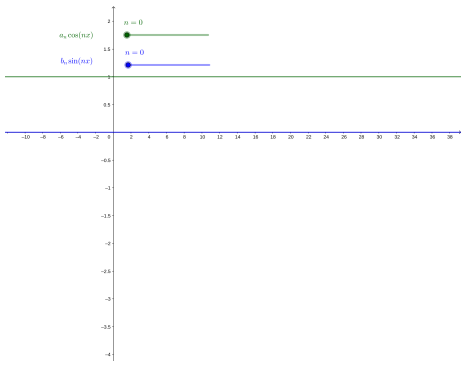


Figure 20.3.1 An applet that allows you to explore the shapes of the Fourier basis functions.

Answer. You should have noticed the following features:

1. All of the functions are sinusoidal, that is, $\cos(mx)$ or $\sin(mx)$ for integer m.
2. The coefficient of the constant term ($\cos(mx)$ for $m = 0$) is $\frac{1}{2}a_0$.
3. The coefficients a_m correspond to cosine functions.
4. The coefficients b_m correspond to sine functions.
5. The subscript m on the coefficients a_m and b_m corresponds to the value m in $\cos(mx)$ or $\sin(mx)$.

20.4 Derivation of Fourier Coefficients

We are now ready to find formulas for the Fourier coefficients a_n and b_n. Using the idea outlined at the start of Section 14.7, the coefficient of each basis element can be obtained from the inner product, i.e. the analogue of the "dot product" of that basis element with the original "vector".

Let's start with the a_n coefficients for $n \neq 0$. The corresponding basis elements are $\cos(nx)$, so we compute

$$\begin{aligned}
&\cos(nx) \cdot f(x) \\
&\quad = \int_0^{2\pi} \cos(nx)\, f(x)\, dx \\
&\quad = \int_0^{2\pi} \cos(nx) \left[\frac{1}{2}a_0 + \sum_{m=1}^{\infty} a_m \cos(mx) \right. \\
&\qquad\qquad \left. + \sum_{m=1}^{\infty} b_m \sin(mx) \right] dx \\
&\quad = \frac{1}{2}a_0 \cancelto{0}{\int_0^{2\pi} \cos(nx)\, dx} \\
&\qquad + \sum_{m=1}^{\infty} a_m \cancelto{\pi\delta_{nm}}{\int_0^{2\pi} \cos(nx)\cos(mx)\, dx}
\end{aligned}$$

$$
\begin{aligned}
&\qquad + \sum_{m=1}^{\infty} b_m \cancelto{0}{\int_0^{2\pi} \cos(nx)\sin(mx)\,dx} \\
&= \sum_{m=1}^{\infty} a_m \pi \delta_{mn} \\
&= \pi a_n
\end{aligned} \tag{20.4.1}
$$

where we see the squared norm of the basis function appear in the next-to-last line. In conclusion,

$$a_n = \frac{1}{\pi}\int_0^{2\pi} \cos(nx)\, f(x)\,dx. \tag{20.4.2}$$

Activity 20.4.1 Finding Fourier Coefficients. Use similar reasoning to obtain the formulas

$$a_0 = \frac{1}{\pi}\int_0^{2\pi} \cos(0x)\ f(x)\,dx = \frac{1}{\pi}\int_0^{2\pi} f(x)\,dx \tag{20.4.3}$$

and

$$b_n = \frac{1}{\pi}\int_0^{2\pi} \sin(nx)\ f(x)\,dx \tag{20.4.4}$$

Solution. For the a_0 term, the corresponding basis element is just the constant function, so we compute

$$
\begin{aligned}
&\cos(0x)\cdot f(x) \\
&\quad = \int_0^{2\pi} \cancelto{1}{\cos(0x)} f(x)\,dx \\
&\quad = \int_0^{2\pi} 1 \left[\frac{1}{2}a_0 + \sum_{m=1}^{\infty} a_m \cos(mx) \right. \\
&\qquad\qquad \left. + \sum_{m=1}^{\infty} b_m \sin(mx)\right] dx \\
&\quad = \frac{1}{2}a_0 \int_0^{2\pi} dx \\
&\qquad + \sum_{m=1}^{\infty} a_m \cancelto{0}{\int_0^{2\pi} \cos(mx)\,dx} \\
&\qquad + \sum_{m=1}^{\infty} b_m \cancelto{0}{\int_0^{2\pi} \sin(mx)\,dx} \\
&\quad = \pi a_0
\end{aligned} \tag{20.4.5}
$$

In conclusion,

$$\frac{1}{2}a_0 = \frac{1}{2\pi}\int_0^{2\pi} f(x)\,dx. \tag{20.4.6}$$

Thus, the term $a_0/2$ in the series represents the average value of f (on the given interval).

We leave the b_n calculation for the reader.

The conventional factor of $\frac{1}{2}$ in the definition of a_0 can now be justified by noting that the factor preceding the integral in (20.4.3) is the same as the factors preceding the integrals in (20.4.2) and (20.4.4).

20.5 Alternative Forms of Fourier Series

There are many different forms of the Fourier series and therefore different formulas for the Fourier series coefficients, depending on the physical context.

We are using the names a_n, b_n, and c_n as the names for the coefficients in every case, below, but of course the *values* of these coefficients and the formulas for finding them are slightly different in each case. Be careful to pair the formula for the coefficient with the form of the Fourier series that you are using, especially if you are pulling formulas from multiple sources. See the activity with hints and example solution below.

The factors that will help you choose the correct form of the Fourier series are:

- The zeros of the trig functions sine and cosine occur when the argument is an integer multiple of 2π, so you will see versions of the formulas both without and with factors of 2π explicitly in the argument:

$$f(\theta) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos n\theta + \sum_{n=1}^{\infty} b_n \sin n\theta \tag{20.5.1}$$

  or

$$f(\theta) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos 2\pi n\theta + \sum_{n=1}^{\infty} b_n \sin 2\pi n\theta \tag{20.5.2}$$

  In the first case, the variable θ runs from 0 to 2π and in the second case, it runs from 0 to 1.

- The argument of special functions like sine, cosine, and exponential must always be dimensionless (see Section 13.8), so if the independent variable has dimensions, it must always be divided by some constant with the same dimensions. The most typical examples are: the independent variable is a (rectangular) spatial dimension like x, in which case it will appear in the formulas divided by a constant length, for example L, which represents the wavelength of the phenomenon

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi nx}{L}\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{2\pi nx}{L}\right) \tag{20.5.3}$$

  or the independent variable is time t, in which case it will appear in the formulas divided by a constant time, for example T, which represents the period of the phenomenon.

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi nt}{T}\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{2\pi nt}{T}\right) \tag{20.5.4}$$

- The integration in the formulas must always be over the period of the phenomenon, e.g. L or T in the examples immediately above.

- Using Euler's formula (see Section 2.6), sines and cosines can always be rewritten as (complex) exponentials. Therefore, there is an exponential form of the Fourier series.

$$f(\theta) = \sum_{n=-\infty}^{\infty} c_n e^{in\theta} \tag{20.5.5}$$

A big advantage of the exponential form is that it is only necessary to use a single sum, although the sum begins at $n = -\infty$ instead of 0 or 1. The trade-off is that you are now in complex-number land. For a real-valued function, the constants c_n and c_{-n} must be complex conjugates of each other. (Why?) This exponential form can also come with and without various dimensions and with or without explicit factors of 2π in the argument, as in the bullets above.

Activity 20.5.1 Formulas for the coefficients of different forms of Fourier series. Starting from the formulas (20.4.2) and (20.4.4) for the coefficients for a_m and b_m, and using any method you know for changing variables in integrals, find formulas for the coefficients for each of the other forms of the Fourier series listed above.

Hint. Don't forget to change the limits in the integrals appropriately. Also, notice that the overall constant factors change in each case.

Answer. As an example, the formulas for the coefficients corresponding to the form (20.5.3) involving the spatial variable x are:

$$a_n = \frac{2}{L}\int_0^L \cos\left(\frac{2\pi nx}{L}\right) f(x)\,dx \tag{20.5.6}$$

$$b_n = \frac{2}{L}\int_0^L \sin\left(\frac{2\pi nx}{L}\right) f(x)\,dx \tag{20.5.7}$$

20.6 Fourier Series Example

Let's consider an example. Suppose $f(x)$ describes a square wave of height C, so that

$$f(x) = C\,\Theta\left(\frac{L}{2} - x\right) = \begin{cases} C & (0 \le x < \frac{L}{2}) \\ 0 & (\frac{L}{2} < x \le L) \end{cases} \tag{20.6.1}$$

where the step function Θ is defined in Section 17.3 (The value of f at the single point $x = L/2$ doesn't matter).

According to the previous sections, we have

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi nx}{L}\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{2\pi nx}{L}\right) \tag{20.6.2}$$

where

$$a_0 = \frac{2}{L}\int_0^{\frac{L}{2}} C\,dx = C, \tag{20.6.3}$$

$$a_n = \frac{2}{L}\int_0^{\frac{L}{2}} \cos\left(\frac{2\pi nx}{L}\right) C\,dx = 0, \tag{20.6.4}$$

$$b_n = \frac{2}{L}\int_0^{\frac{L}{2}} \sin\left(\frac{2\pi nx}{L}\right) C\,dx = \begin{cases} \frac{2C}{\pi n} & (n \text{ odd}) \\ 0 & (n \text{ even}) \end{cases} \tag{20.6.5}$$

Putting this all together,

$$f(x) = C\left(1 + \sum_{\substack{n=1 \\ n\,\text{odd}}}^{\infty} \frac{2}{\pi n} \sin\left(\frac{2\pi nx}{L}\right)\right). \tag{20.6.6}$$

It is instructive to plot the first few terms of this Fourier series and watch the approximation improve as more terms are included, as shown in Figure 20.6.1.

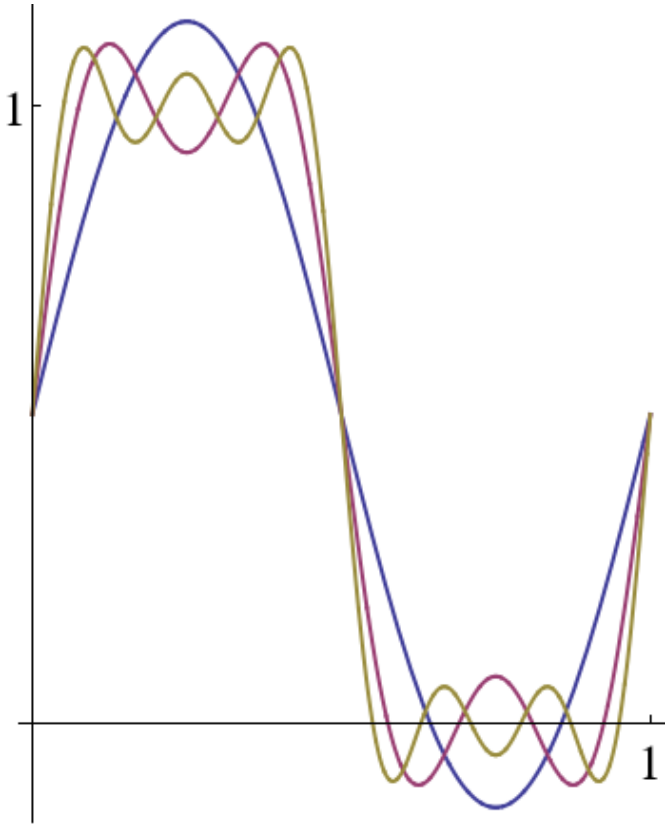


Figure 20.6.1 The first few partial sums in the Fourier series for a step function.

20.7 Fourier Series: Worked Example

Make sure to complete the activity in Section 20.3 before attempting this one.

In this section, we will use the formulas in Section 20.2 to work out an example, the Fourier series for the function $f(x) = -\frac{1}{2} + \sin(x)\sin(2x)$. Then you will plot the individual terms in the Fourier series and their partials sums using an applet.

The formula for the first coefficient a_0 is given in (20.4.3). You can use the Sage code below to calculate the value of this integral.

```
n=0
f=-0.5+sin(x)*sin(2*x)
1/pi*integrate(f*cos(n*x),x,0,2*pi)
```

Using the applet in Figure 20.7.1, set the $a_0/2$ slider to correspond to the value you just calcuated. Compare your approximate Fourier series, containing just one term (shown in green), to the actual function (shown in blue).

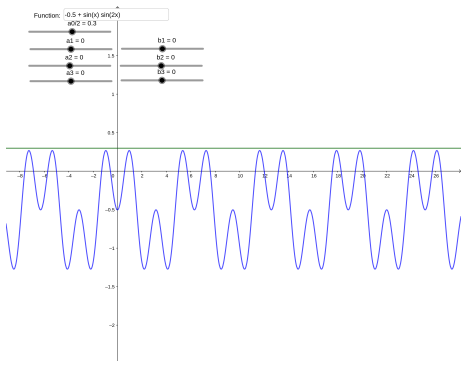


Figure 20.7.1 An applet for manipulating the individual Fourier coefficients.

You should notice that $\frac{1}{2}a_0$ is just the average value of the function. Because the given function is symmetric vertically, this zeroth-order approximation (green) runs across the middle of the graph of the function (blue). In general, the integral in (20.4.3) *defines* what you mean by "the middle".

Now you can alter the Sage code above to compute the other coefficients, using (20.4.2) and (20.4.4) in Section 20.4. After each calculation, move the corresponding slider to the value you obtain, and compare the approximation to the given function.

If you move the sliders one by one, resetting the others to zero, you will see how much each individual term contributes to the Fourier series.

If you don't reset the other sliders, but instead combine the contributions from each slider, the applet plots the sum of the corresponding terms (in green), representing an approximation to the actual function (in blue). In the given example, you should obtain an exact match when you include all of the terms with $n = 0, 1, 2, 3$ (most of which will be 0). In general, there are an infinite number of nonzero terms in the Fourier series; your approximation will get better and better as you include more terms.

20.8 Fourier Series: Exploration

Make sure to complete the activity in Section 20.3 before attempting this one.

Activity 20.8.1 Guessing the Fourier Coefficients. In Figure 20.8.1 below, use the sliders to match the given function (shown in blue) exactly. Use only graphical reasoning. *Hint: Only three of the sliders need to be set to nonzero values.*

When you are done, make a note of any relationship you see between the values of the coefficients and the shape of the graph.

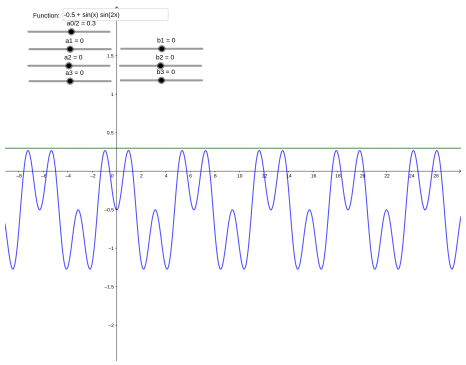


Figure 20.8.1 Use the applet to set the individual Fourier coefficients to try to match the given function.

Hint. Use the Sage code below to calculate the coefficients, if you are having trouble guessing.

Activity 20.8.2 Comparing an exact calculation to your guess. Refer to Section 20.2 to find the formulas for the coefficients in a Fourier series. Use the Sage code below to calculate the coefficients for the function $f(x) = -\frac{1}{2} + \sin(x)\sin(2x)$ used in the previous activity. Check that your calculated coefficients agree with your earlier guess.

```
n=0
f=-0.5+sin(x)*sin(2*x)
1/pi*integrate(f*cos(n*x),x,0,2*pi)
```

Hint. The Sage code calculates a_0. You will need to make minor changes in order to calculate the remaining coefficients.

20.9 Fourier Series: Small Group Activity

Make sure to complete the activity in Section 20.3 before attempting this one.

Activity 20.9.1 Calculating Fourier Coefficients. Refer to Section 20.2 to find the formulas for the coefficients in a Fourier series. Use the Sage code below to calculate the coefficients a_n and b_n for $n = 0, 1, 2, 3$ for the function $-\frac{1}{2} + \sin(x)\sin(2x)$.

```
n=0
f=-0.5+sin(x)*sin(2*x)
1/pi*integrate(f*cos(n*x),x,0,2*pi)
```

The applet in Figure 20.9.1 shows the function $-\frac{1}{2} + \sin(x)\sin(2x)$ (in blue). As you move the sliders, the corresponding Fourier series is also shown (in green). Set the sliders to the values that you calculated. Write as many statements as you can about the relationships between the values of the coefficients and the shape of the graph.

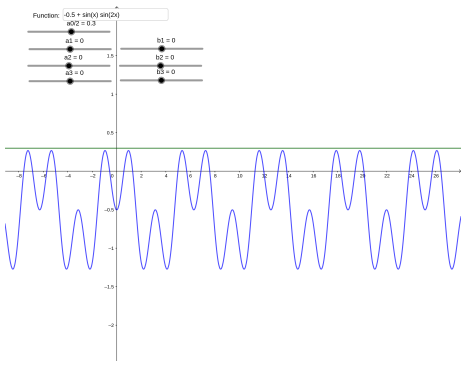


Figure 20.9.1 An applet for manipulating the individual Fourier coefficients.

Solution. (Add wrap-up.)

20.10 The Gibbs Phenomenon

Generally, it is possible to approximate a reasonably smooth function quite well, by keeping enough terms in the Fourier series. However, in the case of a function that has (a finite number of) discontinuities, the Fourier approximation of the function will always "overshoot" the discontinuity. This overshoot phenomenon gets sharper and sharper, i.e. bigger amplitude over a smaller domain, as the number of terms in the approximation is increased.

An example of the Gibbs phenomenon is shown in Figure 20.10.1.

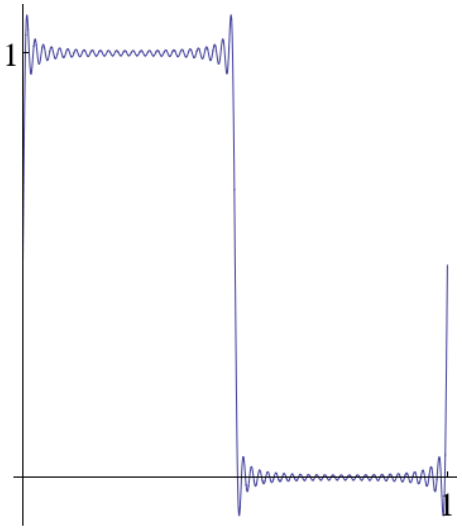


Figure 20.10.1 The Gibbs phenomenon for the Fourier series of a step function. Move the slider to increase the number of terms in the approximation.

20.11 Symmetries

If the function that you are trying to find a Fourier series representation for has a particular symmetry, e.g. if it is symmetric or antisymmetric around the center of the interval for which its defined, then only those basis functions that have the same symmetry will have nonzero coefficients.

FIXME: Add graphs and examples.

Chapter 21

Fourier Transforms

21.1 Gaussians

A Gaussian is a function of the form

$$f(x) = Ne^{-\frac{(x-x_0)^2}{2\sigma^2}}. \tag{21.1.1}$$

Sensemaking 21.1.1 Derivatives of the Gaussian. What do the first and second derivatives of the delta function tell you about the shape of the graph?

Hint. The sign of the first derivative tells you whether the function is increasing (positive derivative) or decreasing (negative derivative). The sign of the second derivative tells you whether the function is concave up (positive second derivative) or concave down (negative second derivative).

The graph below shows the role of the parameters N, x_0, and σ on the shape of the graph.

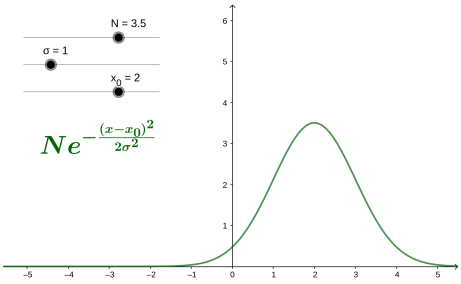


Figure 21.1.1 The graph of a Gaussian with parameters N, x_0, and σ.

Activity 21.1.2 The relationship between the algebraic form of a Gaussian and its shape.. EXPLAIN the relationship between the algebraic form of the Gaussian function and how the parameters N, x_0, and σ control the shape of the graph.

Answer.

- N is an overall multiplicative factor, so increasing (or decreasing) N increases (or decreases) the overall amplitude (height) of the function.
- x_0 appears in the function in the form $x - x_0$, i.e. it appears as a shift in the value of the independent variable, so increasing (or decreasing) x_0 results in a shift of the graph to the right (or left).

- σ occurs in the denominator of a fraction, with the shifted independent variable $x - x_0$ in the numerator. When σ increases (or decreases), the value of the fraction decreases (or increases). This fraction squared appears in anegative exponent, so as the value of the fraction decreases (or increases), the value of the exponential increases (or decreases) which makes the Gaussian wider (or narrower).

21.2 Normalization of the Gaussian

In Section 21.1 we gave a general formula for a Gaussian function with three real parameters. When Gaussian's are used in probability theory, it is essential that the integral of the Gaussian for all x is equal to one, i.e. the area under the graph of the Gaussian is equal to one, so that the total probability of anything happening is one. We can use this condition to find the value of the normalization parameter N in terms of the other two parameters.

Of course, you can use computer algebra to find the value of the integral and/or just look it up online or in a table of integrals, i.e.

$$\int_{-\infty}^{\infty} e^{-x^2}\,dx = \sqrt{\pi} \tag{21.2.1}$$

and use an appropriate substitution. But there is a sweet trick to finding the integral of a Gaussian that is worth knowing.

First, give the name I to the integral you are trying to find

$$I = \int_{-\infty}^{\infty} N e^{-\frac{(x-x_0)^2}{2\sigma^2}}\,dx \tag{21.2.2}$$

Next, find the value of the square of this integral, i.e. this integral times itself. Don't forget to name the "dummy" variables of integration with different names. In this case, we will call the variables x and y, to suggest coordinates in the plane.

$$I^2 = \left(\int_{-\infty}^{\infty} N e^{-\frac{(x-x_0)^2}{2\sigma^2}}\,dx\right)\left(\int_{-\infty}^{\infty} N e^{-\frac{(y-y_0)^2}{2\sigma^2}}\,dy\right) \tag{21.2.3}$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} N^2 e^{-\frac{(x+x_0)^2+(y-y_0)^2}{2\sigma^2}}\,dx\,dy \tag{21.2.4}$$

Finally, taking advantage of the fact that the integration (abstractly) covers the whole two-dimensional plane, we change to polar coordinates, centered at the point (x_0, y_o), using the substitutions

$$(x - x_0)^2 + (y - y_0)^2 = r^2 \tag{21.2.5}$$

$$dx\,dy = r\,dr\,d\phi \tag{21.2.6}$$

to obtain

$$I^2 = \left(\int_0^{2\pi}\left(\int_0^{\infty} N^2 e^{-\frac{r^2}{2\sigma^2}} r\,dr\right)\,d\phi\right) \tag{21.2.7}$$

$$= 2\pi\sigma^2 N^2 \tag{21.2.8}$$

(Note the limits of integration!)

In the final line, the new factor of r in the integrand made it possible to do the integral with the substitution given by $u = \frac{r^2}{2\sigma^2}$ (Details left to the reader. See Section 6.7 for an explanation of substitution in integrals.)

If we want to normalize the function for probability applications, the value of this integral should be equal to one, so we would choose

$$N = \frac{1}{\sqrt{2\pi}\,\sigma} \tag{21.2.9}$$

and the formula for the normalized Gaussian is

$$f(x) = \frac{1}{\sqrt{2\pi}\,\sigma}\, e^{-\frac{(x-x_0)^2}{2\sigma^2}} \tag{21.2.10}$$

In section Section 21.1, you can explore how the parameters N and σ separately affect the shape of the graph of a Gaussian. The normalization condition (21.2.9), relates these two parameters. As a Gaussian gets taller, it must also get narrower in just the right way to keep the area under the curve the same.

21.3 Definition of the Fourier Transform

Consider the (square integrable) function $f(x)$; its Fourier transform is defined by:

$$\mathcal{F}(f) = \tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx}\, f(x)\, dx \tag{21.3.1}$$

The inverse of the Fourier transform is given by:

$$\mathcal{F}^{-1}(\tilde{f}) = f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{ikx}\, dk \tag{21.3.2}$$

To show that the inverse Fourier transform is indeed the inverse operation, start with the right-hand-side of the inverse Fourier transform and insert the definition of the Fourier transform

$$\begin{aligned}
\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{ikx}\, dk &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x')\, e^{-ikx'}\, dx' \right] e^{ikx}\, dk \\
&= \int_{-\infty}^{\infty} f(x') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')}\, dk \right] dx' \\
&= \int_{-\infty}^{\infty} f(x') \delta(x - x')\, dx' \\
&= f(x)
\end{aligned} \tag{21.3.3}$$

where in the second to the last line, we have used the integral representation of the delta function, see Section 17.11, to evaluate the expression in the square brackets.

Conventions.

- We strongly suggest the convention of putting the exponential to the left of the function in the integrand of the Fourier transform (and to the right for the inverse Fourier transform) to highlight the relationship between the Fourier Transform and the quantum mechanics notion of finding the projection of a quantum wavefunction $f(x)$ onto a plane wave (Notice the complex conjugate of the plane wave that turns the ket into a bra).
- We always use the convention of putting a factor of $\frac{1}{\sqrt{2\pi}}$ into the definitions of both the Fourier Transform and its inverse (see below) to make the operations symmetric in this way. This convention is NOT universal; use caution when using other resources.

21.4 Fourier Transform of the Delta Function

The easiest and one of the most important examples of a Fourier Transform is the delta function!

Activity 21.4.1 The Fourier Transform of a Delta Function. Show that the Fourier Transform of the delta function $f(x) = \delta(x - x_0)$ is a constant phase that depends on x_0, where the peak of the delta function is.

Answer.

$$\tilde{\delta}_{x_0}(k) = \frac{1}{\sqrt{2\pi}} e^{-ikx_0} \tag{21.4.1}$$

Solution.

$$\tilde{\delta}_{x_0}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \delta(x - x_0)\, dx \tag{21.4.2}$$

$$= \frac{1}{\sqrt{2\pi}} e^{-ikx_0} \tag{21.4.3}$$

Now, we can use the inverse Fourier transform to derive the important exponential representation of the delta function, (17.11.2).

Activity 21.4.2 The inverse Fourier Transform of a Delta Function. Use the inverse Fourier Transform of the delta function to derive the exponential representation of the delta function.

$$\delta(x - x_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x_0)}\, dk \tag{21.4.4}$$

Solution. We just showed that the Fourier transform of the delta function is a constant phase. This means that the inverse Fourier transform of the phase is a delta function. So, just write down this statement:

$$\delta(x - x_0) = \mathcal{F}^{-1}\left(\frac{1}{\sqrt{2\pi}} e^{-ikx_0}\right) \tag{21.4.5}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{2\pi}} e^{-ikx_0}\right) e^{ikx}\, dk \tag{21.4.6}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x_0)}\, dk \tag{21.4.7}$$

21.5 Properties of the Fourier Transform

In this section, you will find activities that encourage you to prove two important properties of the Fourier transform. These properties are relatively easy to prove. Each activity has a hint if you get stuck and the full solution if you are short on time.

Activity 21.5.1 The Fourier Transform of a Shifted Function. Show that the Fourier transform of a function that is shifted by an amount x_0 is related to the Fourier transform of the original function by a constant phase related to the amount of the shift, i.e.

$$\mathcal{F}(f(x - x_0)) = e^{-ikx_0}\, \mathcal{F}(f(x)). \tag{21.5.1}$$

Hint. Use the substitution $y = x - x_0$ in the definition of the Fourier transform.

Solution. Plug $f(x - x_0)$ into the definition of the inverse Fourier transform

and use the substitution $y = x - x_0$, $dy = dx$. Notice that the (infinite) limits of integration don't change for this substitution.

$$\mathcal{F}(f(x-x_0) = \tilde{f}_{x_0}(k) \tag{21.5.2}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} f(x-x_0)\, dx \tag{21.5.3}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik(y+x_0)} f(y)\, dy \tag{21.5.4}$$
$$= e^{-ikx_0} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-iky} f(y)\, dy \right) \tag{21.5.5}$$
$$= e^{-ikx_0} \tilde{f}(k) \tag{21.5.6}$$
$$= e^{-ikx_0} \mathcal{F}(f) \tag{21.5.7}$$

Activity 21.5.2 The Fourier Transform of a Derivative. Show that the Fourier Transform of the derivative of a function is simply related to the Fourier transform of the original function, as given by the following formula

$$\mathcal{F}\left(\frac{d}{dx} f(x) \right) = \tilde{f}(k)\, ik. \tag{21.5.8}$$

Hint. Take the derivative of both sides of the definition of the inverse Fourier transform with respect to x and simplify. Interpret your simplified expression as the inverse Fourier transform of something.

Solution. The definition of the inverse Fourier transform is given in (21.3.2). Take the derivative of both sides of this equation with respect to x and simplify. Then interpret the expression as an inverse Fourier transform, again using (21.3.2)

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{ikx}\, dk \tag{21.5.9}$$
$$\frac{d}{dx} f(x) = \frac{d}{dx} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{ikx}\, dk \right] \tag{21.5.10}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) \left(\frac{d}{dx} e^{ikx} \right) dk \tag{21.5.11}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) \left(ik\, e^{ikx} \right) dk \tag{21.5.12}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\tilde{f}(k)\, ik \right) e^{ikx}\, dk \tag{21.5.13}$$
$$= \mathcal{F}^{-1} \left(\tilde{f}(k)\, ik \right) \tag{21.5.14}$$
$$\Rightarrow \mathcal{F}\left(\frac{d}{dx} f(x) \right) = \tilde{f}(k)\, ik \tag{21.5.15}$$

21.6 Examples of Fourier Transforms

This section asks you to find the Fourier transform of a cosine function and a Gaussian. Hints and answers are provided, but the details are left for the reader.

Activity 21.6.1 The Fourier Transform of the Cosine. Find the Fourier transform of the cosine function $f(x) = \cos kx$.

Hint. Hint: You must integrate a combination of an exponential and a cosine. It is ALWAYS easier to integrate exponentials, so use the exponential form of the cosine function, (2.6.3).

Answer.

$$\mathcal{F}(\cos kx) = \tilde{f}(k') \tag{21.6.1}$$
$$= \pi\ (\delta(k-k') + \delta(k+k')) \tag{21.6.2}$$

Activity 21.6.2 The Fourier Transform of a Gaussian. Find the Fourier transform of the normalized Gaussian (21.2.10)

$$f(x) = \frac{1}{\sqrt{2\pi}\,\sigma}\, e^{-\frac{(x-x_0)^2}{2\sigma^2}} \tag{21.6.3}$$

Hint. Complete the square in the exponential, see Section A.1, and use the formula for the integral of a Gaussian, see (21.2.1).

Answer.

$$\mathcal{F}\left(\frac{1}{\sqrt{2\pi}\,\sigma}\, e^{-\frac{(x-x_0)^2}{2\sigma^2}}\right) = \tilde{f}(k) \tag{21.6.4}$$
$$= \frac{1}{\sqrt{2\pi}}\, e^{-\frac{k^2\sigma^2}{2}}\, e^{-ikx_0} \tag{21.6.5}$$

Notice that the Fourier transform of a Gaussian is also a Gaussian, but now the factor of σ^2 is in the numerator of the exponential instead of the denominator. How are the shapes of the two Gaussian's related to each other?

21.7 Using Technology to Calculate and Graph Fourier Transforms

The code below will allow you to calculate and plot the Fourier transform of an input function of your choice. The default input function is the Gaussian $f(x) = e^{-x^2}$.

```
pretty_print_default(True)
k=var('k')
f=exp(-x^2)
F=1/sqrt(2*pi)*integrate(f*exp(-i*k*x),x,-infinity,infinity)
F
```

```
plot(F,(k,-5,5))
```

You might also want to try the Fourier transform calculator at Wolfram Alpha.

21.8 Fourier Uncertainties

21.9 Wave Packets

Chapter 22

Waves

22.1 Sums of Harmonic Functions

Harmonic (sinusoidal) functions have many remarkable properties. It is almost always easiest to prove these properties by using Euler's formula to turn the harmonic functions into exponentials, see (2.6.1).

In this section, we explore the effects of adding two harmonic functions. The results here are very useful when you want to describe waves with different algebraic representations. Figure 22.1.1 below shows the graph of $a\cos\phi + b\sin\phi$, subject to the constraint that $a^2 + b^2 = 1$ while Figure 22.1.2 shows the effect of allowing a and b to vary independently.

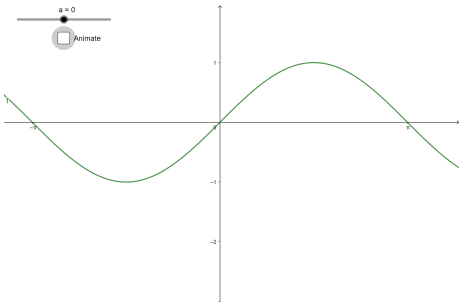


Figure 22.1.1 The graph of $a\cos\phi + b\sin\phi$.

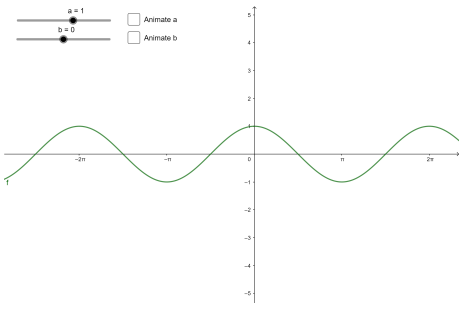


Figure 22.1.2 The graph of $a\cos\phi + b\sin\phi$.

Activity 22.1.1 The sum of two harmonic functions. In the animations above, it looks as if the sum of two harmonic functions is another harmonic function. Show algebraically that this is true, i.e. show that $a\cos\phi + b\sin\phi = r\cos(\phi - \delta)$. Furthermore, find expressions for r and δ in terms of a and b.

Hint. Use Euler's formula (2.6.1)

Answer. $r = \sqrt{a^2 + b^2}$ and $\tan \delta = \frac{b}{a}$.

Chapter 23

Classical Mechanics of Orbits

23.1 Introduction to the Classical Central Force Problem

In this chapter, we will examine a mathematically tractable and physically useful problem - that of two bodies interacting with each other through a *central* force.

Definition 23.1.1 Central Force. A **central force** is a force between two objects that has two characteristics:

1. A central force depends only on the separation distance between the two bodies,
2. A central force points along the line connecting the two bodies.

$\Diamond$

The most common examples of this type of force are those that have $\frac{1}{r^2}$ behavior, specifically the Newtonian gravitational force between two point (or spherically symmetric) masses and the Coulomb force between two point (or spherically symmetric) electric charges. Clearly both of these examples are idealizations - neither ideal point masses or charges nor perfectly spherical mass or charge distributions exist in nature, except perhaps for elementary particles such as electrons. However, deviations from ideal behavior are often small and can be neglected to within a reasonable approximation. (Power series to the rescue!) Also, notice the difference in length scale: the archetypal gravitational example is planetary motion - at astronomical length scales; the archetypal Coulomb example is the hydrogen atom - at atomic length scales.

Our ultimate goal is to solve the equations of motion for two masses m_1 and m_2 subject to a central force acting between them. When you considered this problem in introductory physics, you assumed that one of the masses was so large that it effectively remained at rest while all of the motion belonged to the other object. This assumption works fairly well for the Earth orbiting around the Sun or for a satellite orbiting around the Earth, but in general we are going to have to solve for the motion of *both* objects.

The two solutions to the central force problem - classical behavior exemplified by the gravitational interaction (addressed in this chapter) and quantum behavior exemplified by the Coulomb interaction (addressed in Chapter 24) - are quite different from each other. By studying these two cases together in parallel, we will be able to explore the strong similarities and the important differences between classical and quantum physics.

Two of the unifying themes of this topic are the conservation laws:

1. Conservation of Energy
2. Conservation of Angular Momentum

The classical and quantum systems we will explore both have versions of these conservation laws, but they come up in the mathematical formalisms in different ways.

In the classical mechanics case, we will obtain the equations of motion in three equivalent ways,

1. using Newton's second law,
2. using Lagrangian mechanics,
3. using energy conservation.

so that you will be able to compare and contrast the methods. The Newtonian approach is the most straightforward and naive, but it suggests changes of coordinates that inform the other methods. The Lagrangian and energy conservation approaches are slightly more sophisticated in that they exploit more of the symmetries from the beginning.

We will also consider forces that depend on the distance between the two bodies in ways other than $\frac{1}{r^2}$ and explore the kinds of motion they produce.

23.2 Systems of Particles

Consider a system of n different masses m_i, interacting with each other and being acted on by external forces. We can write Newton's second law for the positions $\vec{\boldsymbol{r}}_i$ of each of these masses with respect to a fixed origin $\boldsymbol{O}$, thereby obtaining a system of equations governing the motion of the masses.

$$\begin{aligned} m_1\frac{d^2\vec{\boldsymbol{r}}_1}{dt^2} &= \vec{\boldsymbol{F}}_1 + 0 + \vec{\boldsymbol{f}}_{12} + \vec{\boldsymbol{f}}_{13} + \ldots + \vec{\boldsymbol{f}}_{1n} \\ m_2\frac{d^2\vec{\boldsymbol{r}}_2}{dt^2} &= \vec{\boldsymbol{F}}_2 + \vec{\boldsymbol{f}}_{21} + 0 + \vec{\boldsymbol{f}}_{23} + \ldots + \vec{\boldsymbol{f}}_{2n} \\ &\vdots \\ m_n\frac{d^2\vec{\boldsymbol{r}}_n}{dt^2} &= \vec{\boldsymbol{F}}_n + \vec{\boldsymbol{f}}_{n1} + \vec{\boldsymbol{f}}_{n2} + \ldots + \vec{\boldsymbol{f}}_{n(n-1)} + 0 \end{aligned} \tag{23.2.1}$$

Here, we have chosen the notation $\vec{\boldsymbol{F}}_i$ for the net external forces acting on mass m_i and $\vec{\boldsymbol{f}}_{ij}$ for the internal force of mass m_j acting on m_i.

In general, each internal force $\vec{\boldsymbol{f}}_{ij}$ will depend on the positions of the particles $\vec{\boldsymbol{r}}_i$ and $\vec{\boldsymbol{r}}_j$ in some complicated way, making (23.2.1) a set of coupled differential equations. To solve the system (23.2.1), we first need to decouple the differential equations, i.e. find an equivalent set of differential equations in which each equation contains only one variable.

The weak form of Newton's third law states that the force $\vec{\boldsymbol{f}}_{12}$ of m_2 on m_1 is equal and opposite to the force $\vec{\boldsymbol{f}}_{21}$ of m_1 on m_2. We see that each internal force appears twice in the system of equations (23.2.1), once with a positive sign and once with a negative sign. Therefore, if we add all of the equations in together, the internal forces will all cancel, leaving:

$$\sum_{i=1}^{n} m_i\frac{d^2\vec{\boldsymbol{r}}_i}{dt^2} = \sum_{i=1}^{n}\vec{\boldsymbol{F}}_i \tag{23.2.2}$$

Notice how surprising equation (23.2.2) is. The right-hand side directs us to add up all of the external forces, each of which acts on a different mass; something you were taught never to do in introductory physics. The left-hand side directs us to add up (the second derivatives of) n "weighted" position vectors pointing from the origin, each to a different mass.

We can simplify the left-hand side of (23.2.2) if we multiply and divide by the total mass $M = m_1 + m_2 + ... + m_n$ and use the linearity of differentiation to "factor out" the derivative operator:

$$\begin{aligned}\sum_{i=1}^{n} m_i \frac{d^2\vec{\boldsymbol{r}}_i}{dt^2} &= M \sum_{i=1}^{n} \frac{m_i}{M} \frac{d^2\vec{\boldsymbol{r}}_i}{dt^2} \\ &= M \frac{d^2}{dt^2} \left(\sum_{i=1}^{n} \frac{m_i}{M} \vec{\boldsymbol{r}}_i \right) \\ &= M \frac{d^2 \vec{\boldsymbol{R}}_{\text{cm}}}{dt^2}\end{aligned} \tag{23.2.3}$$

Definition 23.2.1 Position of the Center of Mass. We recognize (or define) the quantity in the parentheses on the right-hand side of (23.2.3) as the **position vector $\vec{\boldsymbol{R}}_{\text{cm}}$ from the origin to the center of mass of the system of particles**

$$\vec{\boldsymbol{R}}_{\text{cm}} = \sum_{i=1}^{n} \frac{m_i}{M} \vec{\boldsymbol{r}}_i. \tag{23.2.4}$$

◊

With these simplifications, (23.2.2) becomes:

$$M \frac{d^2 \vec{\boldsymbol{R}}_{\text{cm}}}{dt^2} = \sum_{i=1}^{n} \vec{\boldsymbol{F}}_i \tag{23.2.5}$$

which has the form of Newton's 2nd Law for a fictitious particle with mass M sitting at the center of mass of the system of particles and acted on by all of the external forces from the original system.

Definition 23.2.2 Momentum of the Center of Mass. We can define the momentum of the center of mass as the total mass times the time derivative of the position of the center of mass:

$$\vec{\boldsymbol{P}}_{\text{cm}} = M \frac{d\vec{\boldsymbol{R}}_{\text{cm}}}{dt} \tag{23.2.6}$$

◊

If there are no external forces acting, then the acceleration of the center of mass is zero and the momentum of the center of mass is constant in time (conserved)

$$M \frac{d^2 \vec{\boldsymbol{R}}_{\text{cm}}}{dt^2} = \frac{d\vec{\boldsymbol{P}}_{\text{cm}}}{dt} = 0 \tag{23.2.7}$$

Notice that the entire discussion above applies even if all of the internal forces are zero ($\vec{\boldsymbol{f}}_{ij} = 0$), i.e. none of the particles have any way of knowing that the others are even present. Such particles are called **non-interacting**. The position of the center of mass of the system will still move according to (23.2.5).

23.3 Reduced Mass

So far, we have found one decoupled equation to replace (23.2.1). What about the other $n-1$ equations? It turns out that, in general, there is no way to decouple and solve the other equations. Physicists often say, "The n-body problem can not be solved in general." Whenever you are stuck trying to solve a general problem, it often pays to start with simpler examples to build up your intuition. We will make two simplifying assumptions.

1. Assume that there are no external forces acting.
2. Assume that there are only two masses.

The system of equations (23.2.1) reduces to

$$\begin{aligned} m_1 \frac{d^2\vec{\boldsymbol{r}}_1}{dt^2} &= -\vec{\boldsymbol{f}}_{21} \\ m_2 \frac{d^2\vec{\boldsymbol{r}}_2}{dt^2} &= +\vec{\boldsymbol{f}}_{21} \end{aligned} \tag{23.3.1}$$

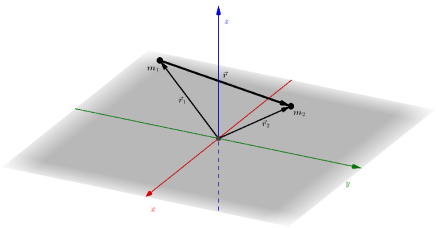


Figure 23.3.1 The position vectors $\vec{\boldsymbol{r}}_1$ and $\vec{\boldsymbol{r}}_2$ for masses m_1 and m_2 and the displacement vector $\vec{\boldsymbol{r}} = \vec{\boldsymbol{r}}_2 - \vec{\boldsymbol{r}}_1$ between them.

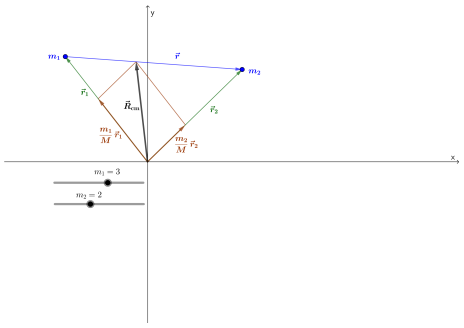


Figure 23.3.2 The position vectors $\vec{\boldsymbol{r}}_1$ and $\vec{\boldsymbol{r}}_2$ for masses m_1 and m_2 and the displacement vector $\vec{\boldsymbol{r}} = \vec{\boldsymbol{r}}_2 - \vec{\boldsymbol{r}}_1$ between them.

Figure 23.3.1 shows the basic geometry of our problem. $\vec{\boldsymbol{r}}_1$ and $\vec{\boldsymbol{r}}_2$ are the position vectors of the two masses measured with respect to an arbitrary coordinate origin $\boldsymbol{O}$. We call the displacement between the two masses $\vec{\boldsymbol{r}}$, the magnitude of this displacement r, and the direction $\hat{\boldsymbol{r}}$. These quantities can be found from $\vec{\boldsymbol{r}}_1$ and $\vec{\boldsymbol{r}}_2$ by

$$\vec{\boldsymbol{r}} = \vec{\boldsymbol{r}}_2 - \vec{\boldsymbol{r}}_1 \tag{23.3.2}$$

$$r = |\vec{\boldsymbol{r}}| = |\vec{\boldsymbol{r}}_2 - \vec{\boldsymbol{r}}_1| \tag{23.3.3}$$

$$\hat{\boldsymbol{r}} = \frac{\vec{\boldsymbol{r}}}{r}. \tag{23.3.4}$$

Because we added the two equations of motion to find the equation of motion for the center-of-mass, we are led now to consider subtracting the equations so as to get $\vec{\boldsymbol{r}} = \vec{\boldsymbol{r}}_2 - \vec{\boldsymbol{r}}_1$. We see that before we subtract, we should multiply the first equation in (23.3.1) by m_2 and the second equation by m_1 so that the factors in front of the second derivative are the same. Subtracting the first equation from the second and regrouping, we obtain:

$$m_1 m_2 \frac{d^2}{dt^2}(\vec{\boldsymbol{r}}_2 - \vec{\boldsymbol{r}}_1) = m_1 m_2 \frac{d^2}{dt^2}(\vec{\boldsymbol{r}}) \tag{23.3.5}$$

$$= (m_1 + m_2)\vec{\boldsymbol{f}}_{21} \tag{23.3.6}$$

or rearranging:

$$\frac{m_1 m_2}{m_1 + m_2}\frac{d^2\vec{\boldsymbol{r}}}{dt^2} = \vec{\boldsymbol{f}}_{21} \tag{23.3.7}$$

Definition 23.3.3 Reduced Mass. The combination of masses

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \tag{23.3.8}$$

is called the **reduced mass**. ◊

Plugging in μ for the reduced mass, (23.3.7) becomes

$$\mu \frac{d^2\vec{\boldsymbol{r}}}{dt^2} = \vec{\boldsymbol{f}}_{21}. \tag{23.3.9}$$

This equation has the same form as Newton's law for a single fictitious mass μ, with position vector $\vec{\boldsymbol{r}}$, moving subject to the force $\vec{\boldsymbol{f}}_{21}$. For the rest of this chapter, when we will talk about "the mass", we will mean this fictitious particle subject to equation (23.3.9).

Note that to solve the original two mass problem we started with, we will need to transform the solutions for $\vec{\boldsymbol{r}}$ back to $\vec{\boldsymbol{r}}_1$ and $\vec{\boldsymbol{r}}_2$.

Activity 23.3.1 Undo Formulas for Center of Mass (Algebra). Find the positions of the two masses in terms of the position of the center of mass and the relative position, i.e. solve for:

$$\vec{r}_1 =$$
$$\vec{r}_2 =$$

Hint. The system of equations (23.2.4) and (23.3.2) is *linear*, i.e. each variable is to the first power, even though the variables are vectors. In this case, you can use all of the methods you learned for solving systems of equations while keeping the variables vector valued, i.e. you can safely ignore the fact that the $\vec{r}$s are vectors while you are doing the algebra *as long as you don't divide by a vector*.

Activity 23.3.2 Undo Formulas for Center of Mass (Geometry). The figure below shows the position vector $\vec{r}$ and the orbit of a "fictitious" reduced mass μ.

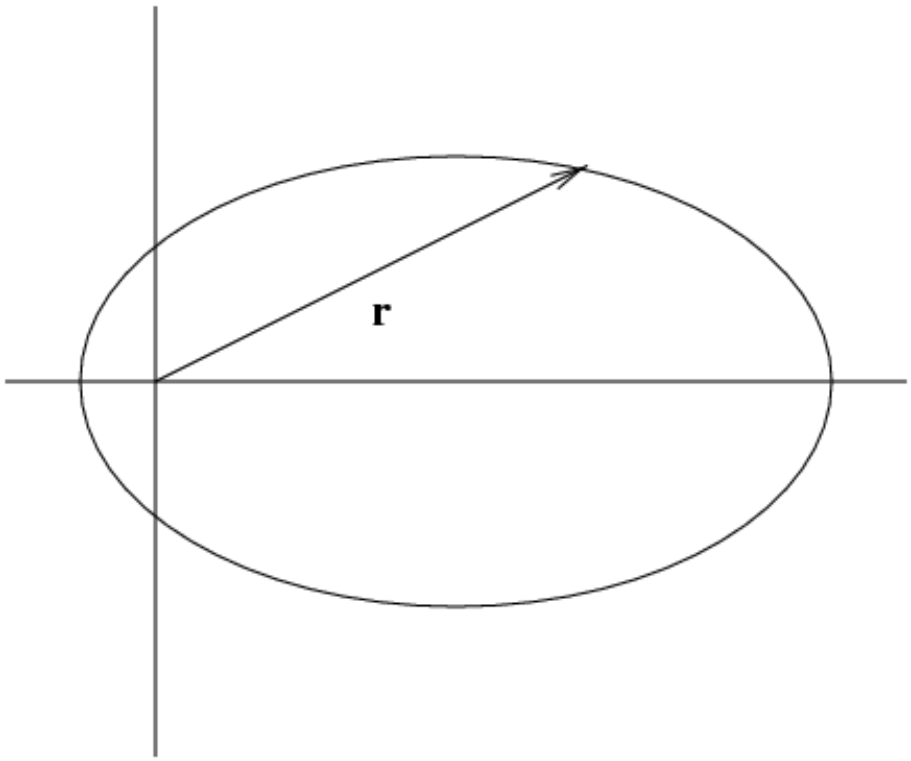


Figure 23.3.4 The position vectors for μ.

1. Suppose $m_1 = m_2$, sketch the position vectors and orbits for m_1 and m_2 corresponding to $\vec{r}$. Describe a common physics example of central force motion for which $m_1 = m_2$.
2. Repeat for $m_2 > m_1$, where the mass difference is neither very large nor very small.

Hint. Think about what you expect in the limiting case $m_2 >> m_1$.

23.4 Central Forces

In the introduction Section 23.1, we defined a central force as satisfying two characteristics. We can now write turn these descriptions of the characteristics into equations:

1. A central force depends only on the separation between the two bodies

$$\vec{\boldsymbol{f}}_{21} = -\vec{\boldsymbol{f}}_{12} = \vec{\boldsymbol{f}}(\vec{\boldsymbol{r}}_2 - \vec{\boldsymbol{r}}_1) \tag{23.4.1}$$

2. A central force points along the line connecting the two bodies

$$\vec{\boldsymbol{f}}_{21} = -\vec{\boldsymbol{f}}_{12} = \vec{\boldsymbol{f}}(\vec{\boldsymbol{r}}_2 - \vec{\boldsymbol{r}}_1) = f(\vec{\boldsymbol{r}})\,\hat{\boldsymbol{r}} \tag{23.4.2}$$

23.5 Angular Momentum

Consider the angular momentum of the reduced mass system $\vec{\boldsymbol{L}} = \vec{\boldsymbol{r}} \times \vec{\boldsymbol{p}} = \vec{\boldsymbol{r}} \times \mu\vec{\boldsymbol{v}}$. How does $\vec{\boldsymbol{L}}$ change with time? We have:

$$\frac{d\vec{\boldsymbol{L}}}{dt} = \frac{d}{dt}\left(\vec{\boldsymbol{r}} \times \mu\vec{\boldsymbol{v}}\right) \tag{23.5.1}$$

$$= \vec{\boldsymbol{r}} \times \mu\dot{\vec{v}} + \cancelto{0}{\vec{\boldsymbol{v}} \times \mu\vec{\boldsymbol{v}}} \tag{23.5.2}$$

$$= \vec{\boldsymbol{r}} \times \mu\vec{\boldsymbol{a}} \tag{23.5.3}$$

$$= \vec{\boldsymbol{r}} \times \vec{\boldsymbol{F}} \tag{23.5.4}$$

$$= \cancelto{0}{r\hat{\boldsymbol{r}} \times f(r)\hat{\boldsymbol{r}}} \tag{23.5.5}$$

$$= 0 \tag{23.5.6}$$

To get from (23.5.1) to (23.5.2), use the product rule, which is valid for cross products as long as you don't change the order of the factors. The second term in (23.5.2) is zero since $\vec{\boldsymbol{v}} \times \vec{\boldsymbol{v}} = 0$. To get from (23.5.4) to (23.5.5), impose the assumption that the force is a central force. The expression (23.5.5) is zero because $r\hat{\boldsymbol{r}} \times \hat{\boldsymbol{r}} = 0$.

Question 23.5.1 *Which of the steps in (23.5.1)-(23.5.6) are valid only for central forces and which are true more generally?*

Definition 23.5.2 Torque. Recall that $\vec{\boldsymbol{r}} \times \vec{\boldsymbol{F}}$ which occurs in (23.5.4) is called the torque $\vec{\boldsymbol{\tau}}$. ◊

To Remember. We have shown that in the case of central forces the time derivative of the angular momentum, and hence the torque, is zero. Therefore:

$$\vec{\boldsymbol{\tau}} = \frac{d\vec{\boldsymbol{L}}}{dt} = 0 \qquad \Longrightarrow \qquad \vec{\boldsymbol{L}} = \text{constant} \tag{23.5.7}$$

Angular momentum is conserved in central force motion.

The central force $\vec{\boldsymbol{F}}(r)$ depends only on the distance of the reduced mass from the center of mass and not on the orientation of the system in space. Therefore, this system is spherically symmetric; it is invariant (unchanged) under rotations. Noether's theorem states that whenever the laws of physics are invariant under a particular motion or other operation, there will be a corresponding conserved quantity. In this case, we see that the conservation of angular momentum is related to the invariance of the physical situation under rotations. Noether's theorem, in general, is most easily discussed using Lagrangian techniques.

23.6 Coordinates

The time has come to choose a coordinate system. We have argued that the reduced mass central force problem is spherically symmetric in nature. Therefore, it will be to our advantage to use spherical coordinates, defined in the spherical coordinates section of Appendix B.1, rather than the more comfortable Cartesian coordinates x, y, and z.

In fact, in the present classical mechanics context, we can do even better. For a central force:

$$F = f(r)\,\hat{\boldsymbol{r}} \tag{23.6.1}$$

the force, and hence the acceleration, is in the radial direction. Therefore, the path of the motion (orbit) will be in the plane determined by the position vector $\vec{\boldsymbol{r}}$ and velocity vector $\vec{\boldsymbol{v}}$ of the reduced mass at any one moment of time. Since there is never a component of force out of this plane, the subsequent motion must remain in the plane. In this plane, choose plane polar coordinates:

$$x = r\cos\phi \tag{23.6.2}$$
$$y = r\sin\phi \tag{23.6.3}$$

Notice that many textbooks choose to call the angle of plane polar coordinates θ. We choose ϕ so that plane polar coordinates can be seen as a cross-section of spherical coordinates through the x, y-plane, i.e. for $\theta = \frac{\pi}{2}$.

23.7 Velocity & Acceleration

Newton's Laws require a knowledge of velocity and acceleration. In Section 23.6, we chose plane polar coordinates, so now we must deal with the problem of how to compute velocity and acceleration as time derivatives of the position vector $\vec{\boldsymbol{r}} = r\hat{\boldsymbol{r}}$ in terms of the coordinates r and ϕ and the basis vectors $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{\phi}}$. A difficulty arises because $\hat{\boldsymbol{r}}$ (and $\hat{\boldsymbol{\phi}}$) are not independent of position and therefore are not independent of time. This problem does not present itself in Cartesian coordinates because $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$ are independent of position. Using the chain rule, the general velocity vector is given by:

$$\vec{\boldsymbol{v}} = \frac{d\vec{\boldsymbol{r}}}{dt} = \frac{d}{dt}(r\,\hat{\boldsymbol{r}}) = \frac{dr}{dt}\,\hat{\boldsymbol{r}} + r\,\frac{d\hat{\boldsymbol{r}}}{dt} \tag{23.7.1}$$

To evaluate (23.7.1), we need the derivatives of $\hat{\boldsymbol{r}}$ (and $\hat{\boldsymbol{\phi}}$) with respect to time.

One method for finding these time derivatives is to exploit the time independence of the Cartesian basis. From Figure 23.7.1, we see that $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{\phi}}$ are given, in terms of $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$, by

$$\begin{aligned}\hat{\boldsymbol{r}} &= \cos\phi\,\hat{\boldsymbol{x}} + \sin\phi\,\hat{\boldsymbol{y}}\\ \hat{\boldsymbol{\phi}} &= -\sin\phi\,\hat{\boldsymbol{x}} + \cos\phi\,\hat{\boldsymbol{y}}\end{aligned} \tag{23.7.2}$$

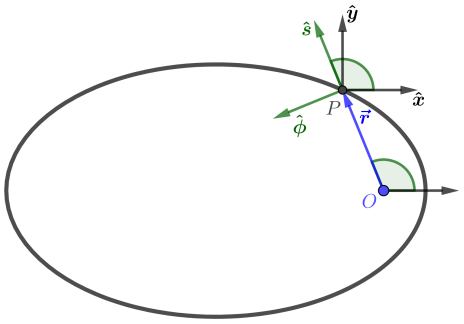


Figure 23.7.1 The polar basis vectors at the point P can be found in terms of the Cartesian basis vectors.

You should recognize this basis change as a rotation performed on the $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$ basis.

$$\begin{pmatrix}\hat{\boldsymbol{r}}\\ \hat{\boldsymbol{\phi}}\end{pmatrix} = \begin{pmatrix}\cos\phi & \sin\phi\\ -\sin\phi & \cos\phi\end{pmatrix}\begin{pmatrix}\hat{\boldsymbol{x}}\\ \hat{\boldsymbol{y}}\end{pmatrix} = R(\phi)\begin{pmatrix}\hat{\boldsymbol{x}}\\ \hat{\boldsymbol{y}}\end{pmatrix} \tag{23.7.3}$$

Using the chain rule, the general velocity vector is given by:

$$\vec{\boldsymbol{v}} = \frac{d\vec{\boldsymbol{r}}}{dt} = \frac{d}{dt}(r\,\hat{\boldsymbol{r}}) = \frac{dr}{dt}\,\hat{\boldsymbol{r}} + r\,\frac{d\hat{\boldsymbol{r}}}{dt} \tag{23.7.4}$$

To evaluate (23.7.1), we need the derivatives of $\hat{\boldsymbol{r}}$ (and $\hat{\boldsymbol{\phi}}$) with respect to time. Using the definitions in (23.7.3) above, we obtain:

$$\begin{aligned}\frac{d\hat{\boldsymbol{r}}}{dt} &= \frac{d}{dt}(\cos\phi\,\hat{\boldsymbol{x}} + \sin\phi\,\hat{\boldsymbol{y}}) \\ &= -\sin\phi\frac{d\phi}{dt}\,\hat{\boldsymbol{x}} + \cos\phi\frac{d\phi}{dt}\,\hat{\boldsymbol{y}} \\ &= \frac{d\phi}{dt}\,\hat{\boldsymbol{\phi}} \\ \frac{d\hat{\boldsymbol{\phi}}}{dt} &= \frac{d}{dt}(-\sin\phi\,\hat{\boldsymbol{x}} + \cos\phi\,\hat{\boldsymbol{y}}) \\ &= -\cos\phi\frac{d\phi}{dt}\,\hat{\boldsymbol{x}} - \sin\phi\frac{d\phi}{dt}\,\hat{\boldsymbol{y}} \\ &= -\frac{d\phi}{dt}\,\hat{\boldsymbol{r}}\end{aligned} \tag{23.7.5}$$

where we have used the Cartesian expressions (23.7.2) for the polar basis vectors in the last equalities of each calculation.

Notice that we have used the convenient notation of putting a dot over a symbol to denote time derivative.

Combining these expressions with equation (23.7.1) gives:

$$\vec{\boldsymbol{v}} = \dot{r}\,\hat{\boldsymbol{r}} + r\dot{\phi}\,\hat{\boldsymbol{\phi}} \tag{23.7.6}$$

Alternatively, in Section 23.8, we use only reasoning about the orthonormality of $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{\phi}}$ to find the same result.

Activity 23.7.1 Acceleration in Polar Coordinates. Taking another derivative of (23.7.6) with respect to time, show that the acceleration is given by

$$\begin{aligned}\vec{\boldsymbol{a}} &= \dot{\vec{v}} \\ &= \left(\ddot{r} - r\dot{\phi}^2\right)\hat{\boldsymbol{r}} + \left(r\ddot{\phi} + 2\dot{r}\dot{\phi}\right)\hat{\boldsymbol{\phi}}\end{aligned} \tag{23.7.7}$$

23.8 Derivatives of Basis Vectors

Differentiating a vector field expressed in terms of the standard, rectangular basis vectors is easy: Just differentiate the coefficients. Why? Because the rectangular basis vectors are constant, that is

$$d\hat{\boldsymbol{x}} = d\hat{\boldsymbol{y}} = d\hat{\boldsymbol{z}} = 0. \tag{23.8.1}$$

However, if the vector field is expressed in terms of curvilinear basis vectors, the product rule must be used! That is, both the coefficients and the basis vectors must be differentiated. So we need to determine the differentials of the basis vectors.

We start with polar coordinates. One could of course express the polar basis $\{\hat{\boldsymbol{r}}, \hat{\boldsymbol{\phi}}\}$ in terms of the rectangular basis $\{\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}\}$ as in Section 23.7 and differentiate, then transform the result back to the original, polar basis. But this calculation can also be done entirely in the polar basis, as we show here.

Recall from Section 1.16 that the position vector in polar coordinates is given by

$$\vec{\boldsymbol{r}} = r\,\hat{\boldsymbol{r}}. \tag{23.8.2}$$

Zapping both sides of (23.8.2) with d and using the product rule yields

$$d\vec{\boldsymbol{r}} = dr\,\hat{\boldsymbol{r}} + r\,d\hat{\boldsymbol{r}}. \tag{23.8.3}$$

Comparing (23.8.3) with the the geometric formula (8.3.1), we conclude that

$$d\hat{\boldsymbol{r}} = d\phi\,\hat{\boldsymbol{\phi}}. \tag{23.8.4}$$

To find $d\hat{\boldsymbol{\phi}}$, we use the product rule together with the orthonormality of the polar basis. Starting from

$$\hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{\phi}} = 1 \tag{23.8.5}$$

we immediately have

$$d\hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{\phi}} + \hat{\boldsymbol{\phi}} \cdot d\hat{\boldsymbol{\phi}} = 2d\hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{\phi}} = 0, \tag{23.8.6}$$

a property that holds for *any* unit vector. Thus, the $\hat{\boldsymbol{\phi}}$ component of $d\hat{\boldsymbol{\phi}}$ must vanish. Similarly, starting from

$$\hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{r}} = 0 \tag{23.8.7}$$

we obtain

$$d\hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{r}} + \hat{\boldsymbol{\phi}} \cdot d\hat{\boldsymbol{r}} = 0 \tag{23.8.8}$$

or equivalently

$$d\hat{\boldsymbol{\phi}} \cdot \hat{\boldsymbol{r}} = -\hat{\boldsymbol{\phi}} \cdot d\hat{\boldsymbol{r}} = -\hat{\boldsymbol{\phi}} \cdot (d\phi\,\hat{\boldsymbol{\phi}}) = -d\phi. \tag{23.8.9}$$

Since we have already shown that the $\hat{\boldsymbol{\phi}}$ component of $d\hat{\boldsymbol{\phi}}$ vanishes, we can conclude that

$$d\hat{\boldsymbol{\phi}} = -d\phi\,\hat{\boldsymbol{r}}. \tag{23.8.10}$$

In particular, if we want the time derivatives of the basis vectors, we can divide (23.8.4) and (23.8.10) by dt to obtain

$$\frac{d\hat{\boldsymbol{r}}}{dt} = \frac{d\phi}{dt}\,\hat{\boldsymbol{\phi}} \tag{23.8.11}$$

$$\frac{d\hat{\boldsymbol{\phi}}}{dt} = -\frac{d\phi}{dt}\,\hat{\boldsymbol{r}} \tag{23.8.12}$$

Extending this argument to spherical coordinates isn't quite as straightforward. It's easy to show that (23.8.4) becomes

$$d\hat{\boldsymbol{r}} = d\theta\,\hat{\boldsymbol{\theta}} + r\,\sin\theta\,d\phi\,\hat{\boldsymbol{\phi}} \tag{23.8.13}$$

using an argument similar to the one above. But determining the angular derivatives (without using rectangular basis vectors) requires a different approach. [1] The result, which could of course also be obtained using rectangular basis vectors, is

$$d\hat{\boldsymbol{\theta}} = -d\theta\,\hat{\boldsymbol{r}} + \cos\theta\,d\phi\,\hat{\boldsymbol{\phi}}, \tag{23.8.14}$$

$$d\hat{\boldsymbol{\phi}} = -\sin\theta\,d\phi\,\hat{\boldsymbol{r}} - \cos\theta\,d\phi\,\hat{\boldsymbol{\theta}}. \tag{23.8.15}$$

[1] One possibility is to use the fact that mixed partial derivatives commute, so that for instance $\dfrac{\partial^2\vec{\boldsymbol{r}}}{\partial\theta\,\partial\phi} = \dfrac{\partial^2\vec{\boldsymbol{r}}}{\partial\phi\,\partial\theta}$, along with the fact that the expression for $d\vec{\boldsymbol{r}}$ in spherical coordinates (see the spherical coordinates section of Appendix B.2) tells us that $\frac{\partial\vec{\boldsymbol{r}}}{\partial\theta} = r\,\hat{\boldsymbol{\theta}}$ and $\frac{\partial\vec{\boldsymbol{r}}}{\partial\phi} = r\sin\theta\,\hat{\boldsymbol{\phi}}$. Another approach is to use differential forms (see for instance Chapter 6 of GDF).

23.9 Kinetic Energy & Angular Momentum

In Section 23.7, we showed that the position and velocity vectors in polar coordinates are given by

$$\vec{\boldsymbol{v}} = \dot{r}\,\hat{\boldsymbol{r}} + r\dot{\phi}\,\hat{\boldsymbol{\phi}} \tag{23.9.1}$$

$$\vec{\boldsymbol{a}} = \left(\ddot{r} - r\dot{\phi}^2\right)\hat{\boldsymbol{r}} + \left(r\ddot{\phi} + 2\dot{r}\dot{\phi}\right)\hat{\boldsymbol{\phi}} \tag{23.9.2}$$

Activity 23.9.1 Find the Kinetic Energy and Angular Momentum in Polar Coordinates. Show that the kinetic energy T of the reduced mass in polar coordinates is given by:

$$T = \frac{1}{2}\mu\left(\dot{r}^2 + r^2\dot{\phi}^2\right) \tag{23.9.3}$$

Similarly, show that the magnitude of the angular momentum $|\vec{\boldsymbol{L}}| = \ell$ of the reduced mass μ is given in polar coordinates by:

$$\ell = \mu r^2\dot{\phi} \tag{23.9.4}$$

Hint. Don't forget that $v^2 = \vec{\boldsymbol{v}}\cdot\vec{\boldsymbol{v}}$. Use the product rule.

Since the angular momentum is a constant in central force problems, it's magnitude ℓ is also constant. Therefore (23.9.4) can be used to rewrite differential equations, getting rid of $\dot{\phi}$'s in favor of the variable r and the constant ℓ.

Kepler's second law says that the areal velocity of a planet in orbit is constant in time. This is equivalent to equation (23.9.4). To see why, read in section 8.3 of Marion and Thornton, page 294, from equation 8.10 to the bottom of the page.

23.10 Equations of Motion: $F = \mu a$

The problem is now to the point where we can write the equations of motion in a form we can solve. However, the importance of the preceding sections cannot be stressed enough. The strategies that we used are important to the success of problem solving in many complicated physics situations. Drawing a picture, exploiting symmetries, choosing a convenient origin, and using the most appropriate coordinate system all combine to make the analysis as easy as possible. These and other tricks should always be regarded as a good beginning to any problem.

Newton's second law, reduced and modified for our specific problem is:

$$f(r)\,\hat{\boldsymbol{r}} = \mu\ddot{\vec{r}} = \mu\left(\left(\ddot{r} - r\dot{\phi}^2\right)\hat{\boldsymbol{r}} + \left(r\ddot{\phi} + 2\dot{r}\dot{\phi}\right)\hat{\boldsymbol{\phi}}\right) \tag{23.10.1}$$

The vector equation breaks up, in polar coordinates, into two coupled differential equations for $r(t)$ and $\phi(t)$:

$$f(r) = \mu(\ddot{r} - r\dot{\phi}^2) \tag{23.10.2}$$

$$0 = \mu(r\ddot{\phi} + 2\dot{r}\dot{\phi}) \tag{23.10.3}$$

(23.10.3) is just the polar coordinate statement of angular momentum conservation, which we have already discussed, i.e.:

$$0 = r\mu(r\ddot{\phi} + 2\dot{r}\dot{\phi}) = \frac{d}{dt}\left(\mu r^2\dot{\phi}\right) = \frac{d\ell}{dt} \tag{23.10.4}$$

(To derive verify the equalities in (23.10.4) it is easiest to work from right to left!) Therefore

$$\mu r^2 \dot{\phi} = \ell = \text{constant} \tag{23.10.5}$$

can be solved for $\dot{\phi}$ and used in (23.10.2) to obtain a messy, second-order ODE for $r(t)$:

$$\ddot{r} = \frac{\ell^2}{\mu^2 r^3} + \frac{1}{\mu} f(r) \tag{23.10.6}$$

In principle, we could now insert the particular form of $f(r)$ we are concerned with, solve (23.10.6) for r as a function of t, and insert this value in (23.10.5) and solve for $\phi(t)$. We would then have solved the equations of motion for r, and ϕ, parameterized by the time t. In practice, for any but the simplest forms of $f(r)$, it is impossible to solve the differential equations analytically. Computers to the rescue! In Section 23.16 you can explore numerical solutions for a $1/r^2$ force.

23.11 Graphs in Polar Coordinates

Functions expressed in polar coordinates can be graphed. For the function $r(\phi)$, for each value of ϕ, an angle measured counterclockwise from the x-axis, plot the distance $r(\phi)$, measured outward from the origin.

For example, conic sections can be described in the form

$$r(\phi) = \frac{\alpha}{1 + \varepsilon \cos(\phi - \delta)}$$

as shown in Figure 23.11.1.

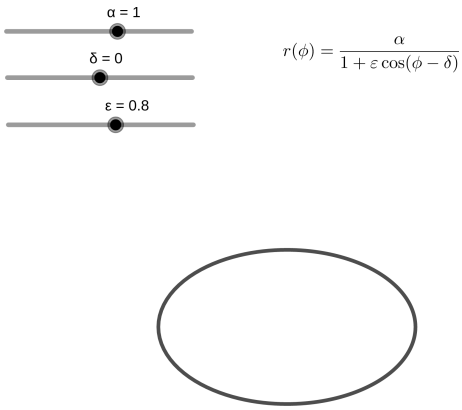


Figure 23.11.1 The polar plot of conic sections.

Activity 23.11.1 Use the visualization above to explore how the shape of a conic section is influenced by the parameters α, ϵ, and δ.

23.12 Shape of the Orbit

In Section 23.10, we reduced the central force problem to a pair of uncoupled ordinary differential equations for the variables r and ϕ as functions of time, i.e. (23.10.5) and (23.10.6).

If we are only interested in the shape of the orbit, we can do something simpler than solving the equations of motion for r and ϕ as functions of t; we can solve for the shape of the orbit, i.e. instead of using the variable t as a

parameter in (23.10.5) and (23.10.6), we will use the variable ϕ and solve for $r(\phi)$, the polar equation for the shape of the orbit.

To do this, we need to change the time derivatives into ϕ derivatives:

$$\frac{d}{dt} = \frac{d\phi}{dt}\frac{d}{d\phi} = \dot{\phi}\frac{d}{d\phi} = \frac{\ell}{\mu r^2}\frac{d}{d\phi} \tag{23.12.1}$$

It turns out that the differential equation which we obtain will be much easier to solve if we also change independent variable from r to

$$u = r^{-1} \tag{23.12.2}$$

(I don't know how to motivate this clever guess.) Therefore,

$$\frac{dr}{dt} = \frac{\ell}{\mu r^2}\frac{dr}{d\phi} = -\frac{\ell}{\mu}\frac{dr^{-1}}{d\phi} = -\frac{\ell}{\mu}\frac{du}{d\phi} \tag{23.12.3}$$

(To verify the second equality, work from right to left.) Then the second derivative is given by

$$\frac{d^2r}{dt^2} = \frac{d}{dt}\frac{dr}{dt} = \frac{\ell}{\mu}u^2\frac{d}{d\phi}\left(-\frac{\ell}{\mu}\frac{du}{d\phi}\right) = -\frac{\ell^2}{\mu^2}u^2\frac{d^2u}{d\phi^2} \tag{23.12.4}$$

Plugging (23.12.2) and (23.12.4) into (23.10.6), dividing through by u^2, and rearranging, we obtain the orbit equation

$$\frac{d^2u}{d\phi^2} + u = -\frac{\mu}{\ell^2}\frac{1}{u^2}\,f\left(\frac{1}{u}\right) \tag{23.12.5}$$

For the special case of inverse square forces $f(r) = -k/r^2$ (spherical gravitational and electric sources), it turns out that the right-hand side of (23.12.5) is constant so that the equation is particularly easy to solve. First, solve the homogeneous equation (with $f(r) = 0$), which is just the harmonic oscillator equation with general solution

$$u_h = A\cos(\phi + \delta) \tag{23.12.6}$$

Add to this any particular solution of the inhomogeneous equation (with $f(r) = -k/r^2$). By inspection, such a solution is just

$$u_p = \frac{\mu k}{\ell^2} \tag{23.12.7}$$

so that the general solution of (23.12.5) for an inverse square force is

$$r^{-1} = u = u_h + u_p = A\cos(\phi + \delta) + \frac{\mu k}{\ell^2} \tag{23.12.8}$$

Then solving for r in (23.12.8) we obtain

$$r = \frac{1}{\frac{\mu k}{\ell^2} + A\cos(\phi + \delta)} = \frac{\frac{\ell^2}{\mu k}}{1 + A'\cos(\phi + \delta)} \tag{23.12.9}$$

This is the equation for a conic section, expressed in polar coordinates. You can explore how the graph of this equation depends on the various parameters in Section 23.11.

23.13 Equations of Motion: Harmonic Oscillator

Using conservation of energy, let's explore the motion of a classical harmonic oscillator.

The statement of energy conservation:

$$E = T + U \tag{23.13.1}$$

becomes

$$E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}(x - x_0)^2 \tag{23.13.2}$$

(23.13.2) can be solved for $\dot{x}$ to give:

$$\dot{x} = \pm\sqrt{\frac{2}{m}\left(E - \frac{1}{2}(x - x_0)^2\right)} \tag{23.13.3}$$

Activity 23.13.1 Explore how the shape of the effective potential (shown in blue) depends on the parameters k and x_0.

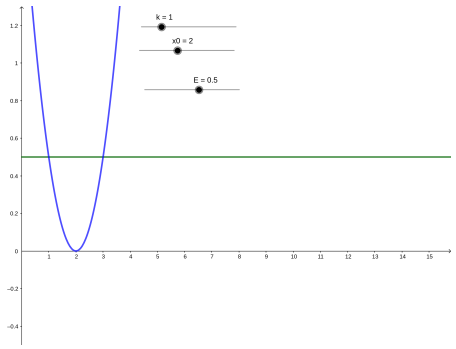


Figure 23.13.1 The effective potential of the classical harmonic oscillator is shown in blue. For a given effective potential, the total energy E, shown in green will determine the resulting motion.

23.14 Equations of Motion: $E = T + U$

Another theoretical tool we can use to arrive at an equation for the orbit is conservation of energy. The central force $\vec{\boldsymbol{F}}$ is conservative and can be derived from a potential $U(r)$ which depends only on the distance from the center of mass (see practice problem [1.2]):

$$\vec{\boldsymbol{F}} = -\vec{\boldsymbol{\nabla}}U = -\frac{\partial U(r)}{\partial r}\,\hat{\boldsymbol{r}} \tag{23.14.1}$$

The statement of energy conservation:

$$E = T + U \tag{23.14.2}$$

becomes, using (23.9.3), (23.9.4), and (23.14.1):

$$E = \frac{1}{2}\mu\dot{r}^2 + \frac{1}{2}\frac{\ell^2}{\mu r^2} + U(r) \tag{23.14.3}$$

(23.14.3) can be solved for $\dot{r}$ to give:

$$\dot{r} = \pm\sqrt{\frac{2}{\mu}\big(E - U(r)\big) - \frac{\ell^2}{\mu^2 r^2}} \tag{23.14.4}$$

(23.14.4) is an equivalent alternative to (23.10.6) as an equation of motion for $r(t)$. You might be surprised that (23.14.4) is a first order differential equation, whereas (23.10.6) is second order. This means that only one initial condition is required for the solution of (23.14.4) whereas two are needed for the solution of (23.10.6). There is nothing surprising going on here. We have already provided the extra information (the extra initial condition) by specifying the constant total energy E.

23.15 Effective Potential

If we compare the equation for the position of a one-dimensional harmonic oscillator (23.13.3)

$$\dot{x} = \pm\sqrt{\frac{2}{m}\big(E - \frac{1}{2}(x - x_0)^2\big)} \tag{23.15.1}$$

from Section 23.13 with the equation for the radial coordinate (23.14.4)

$$\dot{r} = \pm\sqrt{\frac{2}{\mu}\big(E - U(r)\big) - \frac{\ell^2}{\mu^2 r^2}} \tag{23.15.2}$$

$$= \pm\sqrt{\frac{2}{\mu}\big(E - (U(r) + \frac{\ell^2}{2\mu r^2})\big)} \tag{23.15.3}$$

from Section 23.14, we can see an intriguing possibility. If we add together the ordinary potential $U(r)$ and the angular part of the kinetic energy, $-\frac{\ell^2}{2\mu r^2}$, this sum acts the same way in (23.14.4) as the potential does in (23.13.3). Then, we can make a graph analogous to ... and analyze the classical turning points of the motion.

Definition 23.15.1 Effective Potential. The sum of the ordinary potential, $U(r)$ and the angular part of the kinetic energy, $-\frac{\ell^2}{2\mu r^2}$ is called the **effective potential**. ◊

The applet below shows you how the effective potential depends on the parameters: (magnitude of the) angular momentum ℓ, strength of the force k, and reduced mass μ for the case $-\frac{k}{r}$ for spherically symmetric gravitational or electrostatic forces. (Note that the dependence of k on μ for the case of gravitational forces has been ignored.)

Activity 23.15.1 Explore how the shape of the effective potential (shown in black) depends on the parameters ℓ, k, and μ.

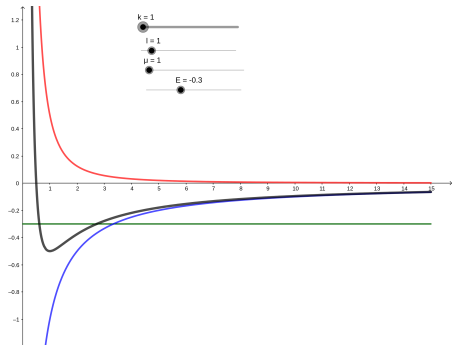


Figure 23.15.2 The effective potential, shown in black is the sum of two terms: the ordinary potential, shown in blue, and the angular part of the kinetic energy, shown in red. For a given effective potential, the total energy E, shown in green will determine the shape of the orbit.

23.16 Effective Potential and Orbits

The animation below shows you the relationship between the orbit and the effective potential. Note that the two superimposed graphs have different axes. The axes for the orbit shape are $x(t)$ and $y(t)$, while the axes for the effective potential are energy plotted vs. the distance $r(t)$ from the center of mass. The two graphs are scaled so that the distance from the center of mass is the same in both graphs, i.e. watch the distance between the orange dot and the two red dots.

Activity 23.16.1 Explore how the orbit is related to the effective potential.

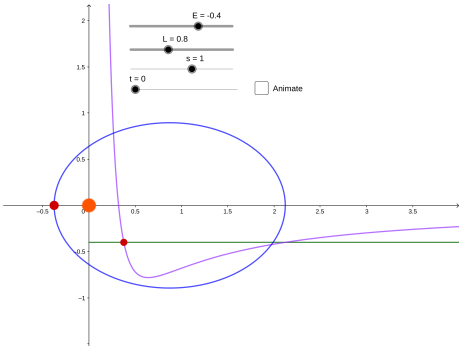


Figure 23.16.1 Orbits and the effective potential.

23.17 Everything Else

You should now work through sections 8.4–8.7 of Taylor. Pay particular attention to the concept of the effective potential.

There are many areas left to explore if you are interested: questions of the stability of orbits under perturbations, the precession of the orbit, and whether it is open or closed. There are many interesting examples, even within our solar system, that show the varied and unique outcomes of central force interactions: Lagrange points, resonant orbits, horseshoe orbits, to name a few. There are also other types of central forces. The repulsive inverse square force was very important to early atomic experiments. Rutherford bombarded a lattice of gold

with alpha particles (helium nuclei). The repulsive electrostatic interaction can be handled easily by our preceding analysis. The theory fit experiment well until the alpha particle energies became high enough to overcome the effective potential and hit the nucleus head-on.

Many of the ideas in our analysis are handled nicely by the Lagrangian formalism which you will study in the Classical Mechanics Capstone. Lagrangian mechanics provides yet another starting point for obtaining the equations of motion. The ideas of symmetry and conservation are more easily recognized and handled within that context, which proves to be very powerful in more complicated situations. When you reach that point, remember some of the techniques we used here and then appreciate the simplicity and beauty provided by the new viewpoint.

Chapter 24

Quantum Mechanics of the Hydrogen Atom

24.1 Introduction to the Quantum Central Force Problem

COMING SOON

24.2 Reduced Mass

It is helpful to consider briefly how the quantum two-body problem separates into an equation governing the center of mass and an equation describing the system around the center of mass, comparing this process to the classical problem. The quantum two-body problem in three dimensions is very messy, but all the essential features of the calculation show up in a simple onedimensional model. So, for simplicity, let's consider a system of two particles, m_1 and m_2, lying on a line at positions x_1 and x_2, and let the interaction between the particles be represented by a potential energy U that depends only on $x = x_1 - x_2$, the separation distance between the particles. Don't worry about how the particles can get past each other on the line—this is a simple toy model; just imagine that they can pass right through each other.

Our first job, as always, is to identify the Hamiltonian H_{op} for the system. Because energies are additive, the kinetic part of the Hamiltonian is just the sum of the kinetic parts for two individual particles and the potential $U(x)$ describes the interaction between them. Therefore the Hamiltonian is

$$H_{\text{op}} = -\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} + U(x) \tag{24.2.1}$$

and the wave function Ψ is a function of the positions of both particles (and of course time) $\Psi = \Psi(x_1, x_2, t)$.

Inspired by our experience with classical two-body systems, we will try rewriting the Hamiltonian (24.2.1) in terms of the center-of-mass coordinate X, given by

$$X = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}$$

and the relative coordinate x. We will use the chain rule of calculus to transform the partial derivatives in (24.2.1) to derivatives with respect to x and X. (Please

see Appendix [A], especially the worked example on plane polar coordinates.) The transformations for first derivatives are:

$$\frac{\partial}{\partial x_1} = \frac{\partial x}{\partial x_1}\frac{\partial}{\partial x} + \frac{\partial X}{\partial x_1}\frac{\partial}{\partial X} = \frac{\partial}{\partial x} + \frac{m_1}{m_1+m_2}\frac{\partial}{\partial X} \tag{24.2.2}$$

$$\frac{\partial}{\partial x_2} = \frac{\partial x}{\partial x_2}\frac{\partial}{\partial x} + \frac{\partial X}{\partial x_2}\frac{\partial}{\partial X} = -\frac{\partial}{\partial x} + \frac{m_2}{m_1+m_2}\frac{\partial}{\partial X} \tag{24.2.3}$$

It is important to note that we cannot simply write equations (24.2.2)–(24.2.3) for the second derivative, which is what we need for the Hamiltonian (24.2.1). To find the second derivative, we must apply the first derivative rules (24.2.2)–(24.2.3) twice:

$$\begin{aligned}\frac{\partial^2}{\partial x_1^2} &= \frac{\partial}{\partial x_1}\frac{\partial}{\partial x_1}\Psi \\ &= \left(\frac{\partial}{\partial x} + \frac{m_1}{m_1+m_2}\frac{\partial}{\partial X}\right)\left(\frac{\partial}{\partial x} + \frac{m_1}{m_1+m_2}\frac{\partial}{\partial X}\right)\Psi \\ &= \frac{\partial^2}{\partial x^2}\Psi + \frac{2m_1}{m_1+m_2}\frac{\partial^2}{\partial x \partial X}\Psi + \left(\frac{m_1}{m_1+m_2}\right)^2\frac{\partial^2}{\partial X^2}\Psi \end{aligned} \tag{24.2.4}$$

$$\begin{aligned}\frac{\partial^2}{\partial x_2^2} &= \frac{\partial}{\partial x_2}\frac{\partial}{\partial x_2}\Psi \\ &= \left(-\frac{\partial}{\partial x} + \frac{m_2}{m_1+m_2}\frac{\partial}{\partial X}\right)\left(-\frac{\partial}{\partial x} + \frac{m_2}{m_1+m_2}\frac{\partial}{\partial X}\right)\Psi \\ &= \frac{\partial^2}{\partial x^2}\Psi - \frac{2m_2}{m_1+m_2}\frac{\partial^2}{\partial x \partial X}\Psi + \left(\frac{m_1}{m_1+m_2}\right)^2\frac{\partial^2}{\partial X^2}\Psi \end{aligned} \tag{24.2.5}$$

Substituting into the Hamiltonian (24.2.1), we obtain for Schrödinger's equation

$$\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x}^2 - \frac{\hbar^2}{2(m_1+m^2)}\frac{\partial^2}{\partial X^2} + U(x)\right)\Psi(X,x,t) = i\hbar\frac{\partial}{\partial t}\Psi(X,x,t) \tag{24.2.6}$$

By transforming to these coordinates, the middle terms in equations (24.2.4) and (24.2.5) have canceled, enabling us to separate the dependence on x from the dependence on X. We can now write

$$\Psi(x,X,t) = \Psi_M(X)\Psi_\mu(x)T(t) \tag{24.2.7}$$

After a separation of variables procedure (see Appendix [B]) on equation (24.2.7), we find that the ordinary differential equation governing the variable X has a simple, recognizable form (see Problem [ProbsC].[14.3b]). The solution has the same form as the free-particle solution to the Schrödinger equation (also called the plane-wave solution to the equation)

$$\Psi_M(X) = e^{iP_X X/\hbar} \tag{24.2.8}$$

where P_X represents the momentum associated with the motion of the center of mass. All observables in quantum mechanics involve the probability density, i.e. terms of the form $\Psi^*\Psi$, so if we are evaluating observables associated with the relative motion, the pure phase contribution from the center-of-mass has no effect. We can therefore ignore the center-of-mass motion and concentrate only on the relative motion.

We have arrived at a conclusion in the quantum analysis of the two-body problem that is similar to our analysis of the classical problem (but for different reasons). We have again replaced the more complicated two-body system with

a fictitious one-body system, involving the relative coordinate and the reduced mass. Once we have solved the problem and found $\Psi_\mu(x)$ and $T(t)$, we can then reverse the procedure in this section to find the wave function $\Psi(x_1, x2, t)$ describing the original two-body system. The analysis in three dimensions is the same, except that we must do the calculation three times, once for each of the rectangular coordinates.

24.3 Schrödinger's Equation in Spherical Coordinates

Schrödinger's equation is

$$H_{\rm op}\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{24.3.1}$$

For one-dimensional waves, the Hamiltonian is

$$H_{\rm op} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + U(x) \tag{24.3.2}$$

In a central potential the role of the second derivative with respect to x is played by the Laplacian operator ∇^2 and the potential energy is a function only on the separation variable $U = U(r)$, making the Hamiltonian:

$$H_{\rm op} = -\frac{\hbar^2}{2\mu}\nabla^2 + U(r) \tag{24.3.3}$$

Because of the parameter r, this problem is clearly asking for the use of spherical coordinates, centered at the origin of the central force.

In rectangular coordinates, we know that the Laplacian ∇^2 is given by:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial z^2}$$

What is the Laplacian in spherical coordinates? Since $\nabla^2 \stackrel{\rm def}{=} \vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{\nabla}}$, combine the spherical coordinate definitions of gradient and divergence

$$\vec{\boldsymbol{\nabla}}V = \frac{\partial V}{\partial r}\,\hat{\boldsymbol{r}} + \frac{1}{r}\frac{\partial V}{\partial\theta}\,\hat{\boldsymbol{\theta}} + \frac{1}{r\sin\theta}\frac{\partial V}{\partial\phi}\,\hat{\boldsymbol{\phi}} \tag{24.3.4}$$

$$\vec{\boldsymbol{\nabla}}\cdot\vec{v} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 v_r\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\, v_\theta\right) + \frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial\phi} \tag{24.3.5}$$

to obtain:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{24.3.6}$$

For convenience, we will give the combination of angular derivatives which appears in (24.3.6) a new name:

$$L_{\rm op} \stackrel{\rm def}{=} -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{24.3.7}$$

Notice the conventional factor of $-\hbar^2$. $\hbar$ is a constant, 1.05459×10^{-27} ergsec $= 6.58217\times10^{-16}$ eV-sec. Notice that the dimensions of $\hbar$ are those of angular momentum. With this definition, (24.3.6) becomes:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}L_{\rm op}^2 \tag{24.3.8}$$

24.4 Separation of Variables on a Ring

To begin our study of the properties of the solutions of Schrödinger's equation in cases with spherical symmetry, we first consider the simpler case of the motion of a quantum particle of mass μ confined to move on a ring of constant radius r_0. As with classical orbits, let's assume that the ring lies in the (x, y)-plane, so that in spherical coordinates $\theta = \frac{\pi}{2} = \text{const}$. Then, since Ψ is independent of r and θ, derivatives with respect to those variables give zero and Schrödinger's equation from Section 24.3 reduces to

$$\begin{aligned} i\hbar\frac{\partial\Psi}{\partial t} &= H_{\text{op}}\Psi \\ &= -\frac{\hbar^2}{2\mu}\frac{1}{r_0^2}\frac{\partial^2}{\partial\phi^2}\Psi + U(r_0)\Psi \end{aligned} \tag{24.4.1}$$

Redoing the separation of variables procedure of Section 18.5, and assuming that $\Psi = T(t)\Phi(\phi)$ only, we obtain the following separated ordinary differential equations

$$\frac{d^2\Phi}{d\phi^2} = -\frac{2I}{\hbar^2}\left(E - U(r_0)\right)\Phi \tag{24.4.2}$$

$$\frac{dT}{dt} = -\frac{i}{\hbar}ET \tag{24.4.3}$$

where we have used the substitution $\mu r_0^2 = I$, in which I would be the moment of inertia of a classical particle of mass μ traveling in a ring of radius r_0 about the center-of-mass.

Alternatively, we could have obtained equations (24.4.2) and (24.4.3) from the results of our original separation of variables procedure (18.5.9), (18.5.15), (18.5.17), (18.5.18), by restricting the variables r and θ to the equator, noticing that the functions R and P are therefore constant, and by finding that equation (18.5.15) reduces to:

$$A = \frac{2\mu}{\hbar^2}(E - U(r_0))r_0^2 \tag{24.4.4}$$

and equation (18.5.17) then reduces to:

$$B = -\frac{2\mu}{\hbar^2}(E - U(r_0))r_0^2. \tag{24.4.5}$$

24.5 Motion on a Ring

Now we want to solve (24.4.2) for $\Phi(\phi)$ obtained from the separation of variables procedure in Section 24.4 for a quantum mechanical particle confined to a ring. Since the coefficient of Φ on the right-hand-side of (24.4.2) is a constant

$$\sqrt{\frac{2I}{\hbar^2}(E - U(r_0))} = \text{constant} \tag{24.5.1}$$

this equation is identical to the equation for an undamped harmonic oscillator, with a solution basis that we can choose to be either sines and cosines or imaginary exponentials. For reasons that will become clear later, we will choose exponentials

$$\Phi_m(\phi) \stackrel{\text{def}}{=} N\, e^{im\phi} \tag{24.5.2}$$

where

$$m = \pm\sqrt{\frac{2I}{\hbar^2}(E - U(r_0))} \tag{24.5.3}$$

and N is a normalization constant.

There is no spatial "boundary" on the ring on which we can impose boundary conditions. However, there is one very important property of the wave function that we can invoke: it must be single-valued. The variable ϕ is geometrically an angle, so that $\phi + 2\pi$ is physically the same point as ϕ. If we go once around the ring and return to our starting point, the value of the wave function must remain the same. Therefore the solutions must satisfy the periodicity condition $\Phi_m(\phi + 2\pi) = \Phi_m(\phi)$. This is impossible unless m is real so that the solutions are oscillatory, i.e. $E - U(r_0) > 0$. Furthermore, the solutions must have the correct period, i.e.

$$m \in \{0, \pm 1, \pm 2, ...\}. \tag{24.5.4}$$

The quantum number m is called the azimuthal or magnetic quantum number. Note that the solution permits both positive and negative values of m as well as zero.

Solving (24.5.3) for the possible eigenvalues of energy, we obtain

$$E_m = \frac{\hbar^2}{2I}\, m^2 + U(r_0) \tag{24.5.5}$$

For this simplified ring problem, we can choose the potential energy $U(r_0)$ to be zero, but we will have to remember that we should not make this choice when we are working on the full hydrogen atom problem. There is a degeneracy that arises in this calculation. Note that the wave functions corresponding to $+|m|$ and $-|m|$ have the same energy but, (as we will see in Section 24.7), represent different states of the motion.

This is a one-dimensional problem, just like the problem of a particle-in-a-box (now using the independent variable ϕ instead of x) and the solutions have the same oscillatory form. Everything that you learned about a particle-in-a-box is immediately applicable here. As in that problem, the energy eigenvalues are discrete because of a boundary condition. The only differences that arise come from the different boundary conditions. In the ring case, the appropriate boundary condition is periodicity, since ϕ is a physical angle. Therefore, the eigenstates have to fit an integer number of wavelengths into the ring and the energy eigenvalues are degenerate. For a particle-in-a-box, $\Psi(x) = 0$ at the boundaries, appropriate to an infinite potential. Therefore, the eigenstates can fit a half integer number of wavelengths into the box and the energy eigenvalues are not degenerate.

24.6 Normalization of States on a Ring

In Section 24.5, we found the energy and angular momentum eigenstates for a quantum particle on a ring to be

$$\Phi_m(\phi) \stackrel{\text{def}}{=} N\, e^{im\phi} \tag{24.6.1}$$

where

$$m \in \{0, \pm 1, \pm 2, ...\} \tag{24.6.2}$$

and N is a normalization constant.

As usual, we choose the normalization N in (24.5.2) so that, if the particle is in an eigenstate, the probability of finding it somewhere on the ring is unity.

$$1 = \int_0^{2\pi} \Phi_m^*(\phi)\,\Phi_m(\phi)\,r_0\,d\phi \tag{24.6.3}$$

$$= \int_0^{2\pi} N^* e^{-im\phi}\,N e^{im\phi}\,r_0 d\phi \tag{24.6.4}$$

$$= 2\pi r_0 |N|^2 \tag{24.6.5}$$

$$\Rightarrow \quad N = \frac{1}{\sqrt{2\pi r_0}} \tag{24.6.6}$$

where we have chosen the arbitrary phase in N to be one.

24.7 Angular Momentum of the Particle on a Ring

Classically, a particle moving in a circle has an angular momentum perpendicular to the plane of the circle, which for a ring in the x, y–plane would be in the z direction. Since angular momentum is defined by $\vec{\boldsymbol{L}} = \vec{\boldsymbol{r}} \times \vec{\boldsymbol{p}}$. To make the transition to quantum mechanics, we replace p_x and p_y by their operator equivalents:

$$L_z = xp_y - yp_x \Longrightarrow \hat{L}_z = x\frac{\hbar}{i}\frac{\partial}{\partial y} - y\frac{\hbar}{i}\frac{\partial}{\partial x} \tag{24.7.1}$$

Using a straightforward application of the chain rule (see Practice Problems, below) to replace the Cartesian partial derivatives with their polar representations, we obtain

$$\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial \phi} \tag{24.7.2}$$

The effect of operating on the ring eigenfunctions with this operator is:

$$\frac{\hbar}{i}\frac{\partial}{\partial \phi}\left(\frac{1}{\sqrt{2\pi}}e^{im\phi}\right) = m\hbar\left(\frac{1}{\sqrt{2\pi}}e^{im\phi}\right) \tag{24.7.3}$$

The energy eigenfunctions $\Phi_m(\phi)$ are thus also eigenfunctions of $\hat{L}_z$ with eigenvalues $m\hbar$. Because the $\Phi_m(\phi)$ are eigenfunctions of both energy and angular momentum, we can make simultaneous determinations of the eigenvalues of energy and angular momentum.

Considering the angular momentum helps us understand the degeneracy of the eigenfunctions with respect to energy. The $\pm m$ degeneracy of the energy eigenstates corresponds to $L_z = +m\hbar$ and $L_z = -m\hbar$. That is, the two degenerate states represent particles rotating in opposite directions around the ring.

For a classical particle rotating in a circular path in the x, y-plane, the kinetic energy is $T = \frac{1}{2}I\omega^2 = L_z^2/2I$, where I is the rotational inertia (moment of inertia). The rotational inertia of a single particle of mass μ moving in a circle of radius r_0 is $I = \mu r_0^2$. The Hamiltonian for the system is thus

$$H = T + U = \frac{L_z^2}{2I} + U = \frac{\hbar^2}{2\mu r_0^2}\frac{\partial^2}{\partial \phi^2} + U_0 \tag{24.7.4}$$

It is apparent from this approach that the energy and the angular momentum have simultaneous eigenvalues because they are commuting operators. Clearly $[L_z^2, L_z] = 0$, so that E and L_z have the same eigenfunctions. Therefore, we

see that (24.4.2) and (24.7.3) are the position-space representations of the eigenvalue equations

$$\hat{H}|m\rangle = E_m|m\rangle \tag{24.7.5}$$

$$\hat{L}|m\rangle = \hbar m|m\rangle \tag{24.7.6}$$

Because the Φ_m are simultaneous eigenstates of both $\hat{H}$ and $\hat{L}_z$, it is possible to make simultaneous measurements of both the energy and the z-component of angular momentum.

In setting up the problem of the particle on the ring, we constrained the motion to the x, y-plane, so that the angular momentum vector is in the z direction. However, according to quantum mechanics (yet another form of the Heisenberg uncertainty relationships) it is not possible to know the direction of the angular momentum vector. Our knowledge of the angular momentum vector is limited to its length and any one component. If the vector lies along the z-axis, then we would know all three of its components (the x and y components being zero). We'll see how the three-dimensional problem solves this contradiction.

24.8 Time Dependence of Ring States

We know, from the theory of Fourier series, that we can write any initial probability distribution, which is necessarily periodic, as a sum of the energy eigenstates:

$$\Phi(\phi) = \sum_{m=-\infty}^{\infty} c_m \Phi_m(\phi) = \sum_{m=-\infty}^{\infty} c_m \left(\frac{1}{\sqrt{2\pi r_0}} e^{im\phi} \right) \tag{24.8.1}$$

where, for the probability distribution to be normalized, we must have:

$$\sum_{m=-\infty}^{\infty} |c_m|^2 = 1 \tag{24.8.2}$$

To find the time evolution of the eigenstates $\Phi_m(\phi)$, we must solve the t equation (24.4.3). Since, for each Φ_m, we have now found the value of the constant $E = E_m$, given by (24.5.5), we can solve (24.4.3) trivially:

$$T(t) = e^{-\frac{\hbar}{i} E_m t} \tag{24.8.3}$$

A deep theorem in the theory of partial differential equations states that if you have found an expansion of the initial probability density in terms of the eigenstates of the Hamiltonian, then the time evolution of that probability density is simply obtained by multiplying each eigenstate individually by the appropriate time evolution:

$$\Phi(\phi, t) = \sum_{m=-\infty}^{\infty} c_m \Phi_m(\phi) e^{-\frac{\hbar}{i} E_m t} \tag{24.8.4}$$

BE CAREFUL! There are an infinite number of different values for the energy, depending on the eigenstate of the Hamiltonian. It is incorrect to multiply the initial state (24.8.1) by a single over-all exponential time factor. Each term in the series gets its own time evolution.

24.9 Visualization of States on a Ring

The applet below displays the real and imaginary parts of the wave function

$$\psi = \sum_m (c_m + id_m)\, e^{im\phi} e^{-im^2 t}$$

as well as the probability density $|\psi|^2$.

Activity 24.9.1 Explore how the ring state is made up out of a linear combination of basis states.

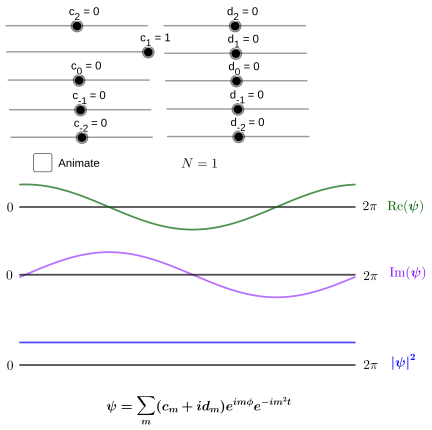


Figure 24.9.1 Move the sliders to visualize linear combinations of eigenstates on the ring. The figure shows plots of the real and imaginary parts of the wave function Reψ, Imψ, and the probablity density $|\psi|^2$. Click on the button for an animation that demonstrates the time dependence.

24.10 Motion on a Sphere

We will now relax the restriction that the mass be confined to the ring and, instead, let it range over the surface of a sphere of radius r_0. The results of this analysis yield predictions that can be successfully compared with experiment for molecules and nuclei that rotate more than they vibrate. For this reason, the problem of a mass confined to a sphere is often called the rigid rotor problem. Furthermore, the solutions that we will find for (18.5.17)–(18.5.18) and, called spherical harmonics, will occur whenever one solves a partial differential equation that involves spherical symmetry.

Following the techniques in Section 24.4, you should be able to write down the Schrödinger equation for a particle restricted to a sphere and use the separation of variables procedure to obtain an equivalent set of ordinary differential equations. One of the equations you obtain will be (18.5.18), with solutions exactly as we found them for the ring in Section 24.5. The other equation will be (18.5.17) with slightly different labels for the unknown constant, i.e.

$$\left(\sin\theta \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) - A\sin^2\theta - m^2\right) P(\theta) = 0 \qquad (24.10.1)$$

where m is a known integer and A is an unknown constant.

A straightforward change of variables (see Section 24.11) turns (24.10.1) into (24.11.6), i.e.

$$\frac{\partial^2 P}{\partial z^2} - \frac{2z}{1-z^2}\frac{\partial P}{\partial z} - \frac{A}{1-z^2}P - \frac{m^2}{(1-z^2)^2}P = 0 \tag{24.10.2}$$

This equation is the Associated Legendre's Equation. For any given integer value of m, it is a Sturm-Liouville equation Section 19.1. The solutions are called Associated Legendre Functions. When the eigenvalue A takes the special form $A = -\ell(\ell+1)$ and for $|m| \leq \ell$, the solutions $P_\ell^m(z)$ form a basis for any sufficiently smooth function on the interval $-1 \leq z \leq 1$ that does not blow up at the endpoints. More information about Associated Legendre functions can be found in Section 19.6 and, of course, online.

If you recognize a known Sturm-Liouville equation, you can always just look up the solutions, called **special functions**. They arise from particular geometric situations, so knowing where the equation comes from will help with guessing which equation it is. But, if you'd like to learn more about how to solve a Sturm-Liouville problem that is unknown or that you don't recognize, you can find an example of using the power series method to solve Legendre's equation (the special case $m = 0$) in Section 16.2 and details about how to use the solutions, called Legendre polynomials, to make an eigenfunction expansion (a generalization of Fourier series) in Chapter 19.

Notice that we have undone the change of coordinates in the Associated Legendre Function by making the replacement $z \to \cos\theta$.

A complete basis of eigenstates for a quantum particle confined to the surface of a sphere (or for the angular part of any PDE involving the Laplacian in spherical coordinates) can be found from multiplying any basis state $\Phi_m(\phi)$ with any basis state $P_\ell^m(\cos\theta)$, subject to the restrictions ℓ is a non-negative integer, m is an integer (positive, negative, or zero), and $m \leq \ell$. Properly normalized, these functions are called spherical harmonics.

$$|\ell, m\rangle \doteq Y_\ell^m(\theta, \phi) \tag{24.10.3}$$

$$= (-1)^{(m+|m|)/2}\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\,P_\ell^m(\cos\theta)\,e^{im\phi} \tag{24.10.4}$$

See Section 19.7 for more details about the algebra and Section 19.8 for some interactive visualizations.

24.11 Change of Variables

Since we have solved the ϕ equation (18.5.18) and found the possible values of the separation constant $\sqrt{B} = m \in \{0, \pm 1, \pm 2, ...\}$, the θ equation becomes an eigenvalue/eigenfunction equation for the unknown separation constant A and the unknown function $P(\theta)$.

$$\left(\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - A\sin^2\theta - m^2\right)P(\theta) = 0 \tag{24.11.1}$$

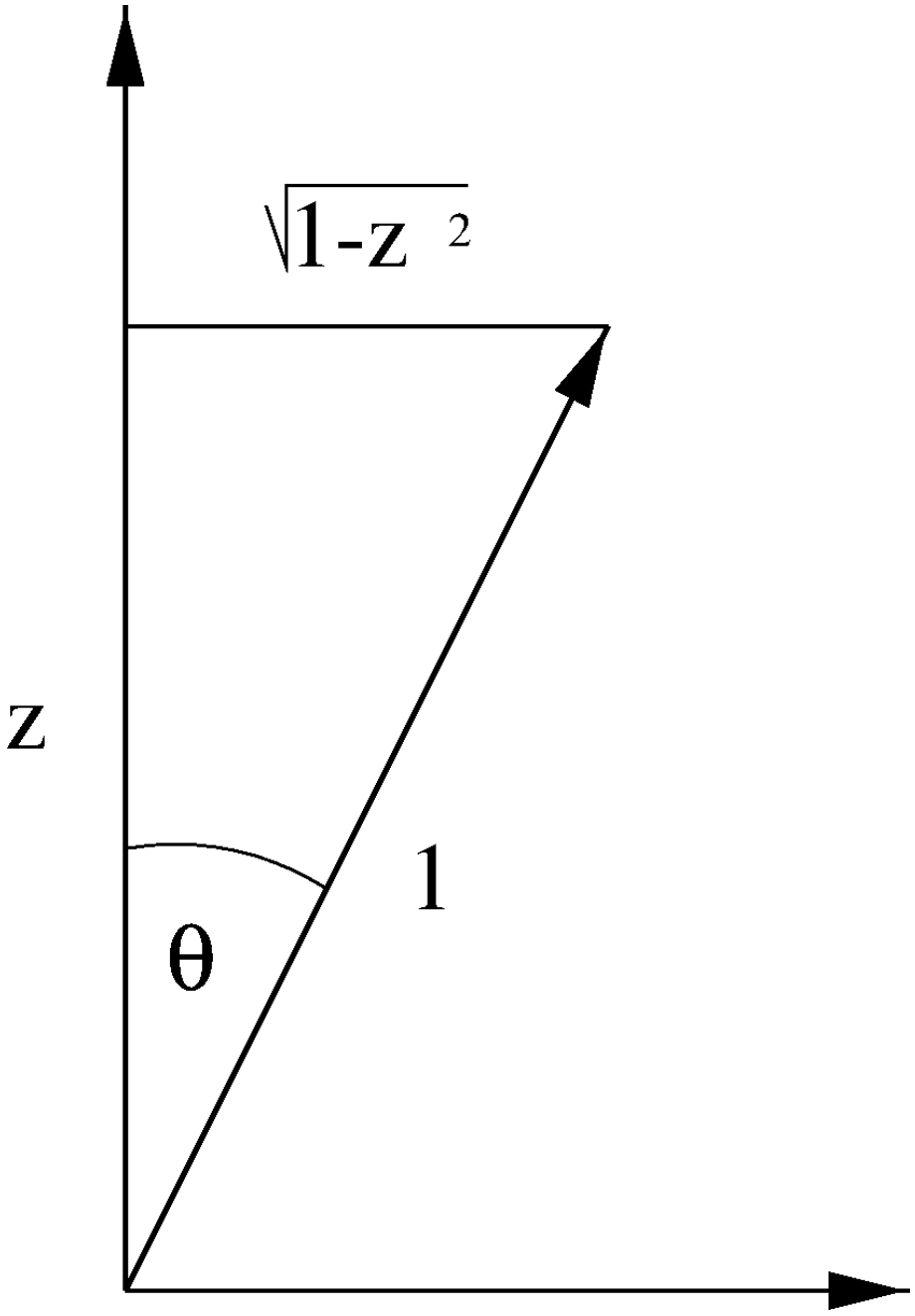


Figure 24.11.1 Relationship between z and θ.

We start with a change of independent variable $z = \cos\theta$ where z is the usual rectangular coordinate in three-space. As θ ranges from 0 to π, z ranges from 1 to -1. We see from Figure 24.11.1 that:

$$\sqrt{1-z^2} = \sin\theta \tag{24.11.2}$$

Using the chain rule for partial derivatives, we have:

$$\frac{\partial}{\partial\theta} = \frac{\partial z}{\partial\theta}\frac{\partial}{\partial z} = -\sin\theta\frac{\partial}{\partial z} = -\sqrt{1-z^2}\frac{\partial}{\partial z} \tag{24.11.3}$$

Notice, particularly, the last equality: we are trying to change variables from θ to z, so it is important to make sure we change **all** the θ's to z's. Multiplying

by $\sin\theta$ we obtain:

$$\sin\theta\frac{\partial}{\partial\theta} = -\left(1-z^2\right)\frac{\partial}{\partial z} \tag{24.11.4}$$

Be careful finding the second derivative; it involves a product rule:

$$\begin{aligned}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) &= \left(1-z^2\right)\frac{\partial}{\partial z}\left(\left(1-z^2\right)\frac{\partial}{\partial z}\right)\\ &= \left(1-z^2\right)^2\frac{\partial^2}{\partial z^2} - 2z\left(1-z^2\right)\frac{\partial}{\partial z}\end{aligned} \tag{24.11.5}$$

Inserting (24.11.2) and (24.11.5) into (24.11.1), we obtain a standard form of the Associated Legendre's equation:

$$\frac{\partial^2 P}{\partial z^2} - \frac{2z}{1-z^2}\frac{\partial P}{\partial z} - \frac{A}{1-z^2}P - \frac{m^2}{(1-z^2)^2}P = 0 \tag{24.11.6}$$

In Section 16.2 and Section 19.6, we will solve this equation. After we have found the eigenfunctions $P(z)$, we will substitute $z = \cos\theta$ everywhere to find the eigenfunctions of the original equation (24.11.1).

Appendix A

Standard Algebra Strategies

A.1 Completing the Square

An important algebraic technique is known as **completing the square**. For example, when trying to identify the shape of the curve satisfying

$$x^2 - 6x + y^2 = 16 \tag{A.1.1}$$

we can start by noticing the terms $x^2 + y^2$, which suggests that this implicit equation might describe a circle. The equation for a circle involves the sum of squares, so we need to find a way to convert the terms $x^2 - 6x$ into a perfect square. That is, we'd like to replace these terms by something of the form $(x - h)^2$. Expanding, we have

$$(x - h)^2 = x^2 - 2hx + h^2 \tag{A.1.2}$$

so it is clear that we should set $h = 3$. What about the missing term $h^2 = 9$? Take it from the constant term 16! Explicitly, since

$$(x - 3)^2 = x^2 - 6x + 9 \tag{A.1.3}$$

we have

$$16 = x^2 - 6x + y^2 = \big((x - 3)^2 - 9\big) + y^2 \tag{A.1.4}$$

or in other words

$$(x - 3)^2 + y^2 = 25 \tag{A.1.5}$$

which is the equation of a circle of radius 5 centered at the point $(3, 0)$.

This example demonstrates the technique known as **completing the square**. Given an expression of the form

$$Q = ax^2 + bx \tag{A.1.6}$$

we'd like to eliminate the linear term. Reasoning along similar lines as above, we have

$$\begin{aligned} Q &= a\left(x^2 + \frac{b}{a}x\right) = a\left(x^2 + \frac{b}{a}x + \frac{b^2}{4a^2} - \frac{b^2}{4a^2}\right) \\ &= a\left(x + \frac{b}{2a}\right)^2 - \frac{b^2}{4a} \end{aligned} \tag{A.1.7}$$

Completing the square is the technique used to prove the **quadratic formula**, see Section A.2.

A.2 The Quadratic Formula

Definition A.2.1 The Quadratic Formula. The **quadratic formula** gives the solution of the second-order polynomial equation

$$ax^2 + bx + c = 0 \tag{A.2.1}$$

i.e.

$$x = \frac{1}{2a}\left\{-b \pm \sqrt{b^2 - 4ac}\right\} \tag{A.2.2}$$

◊

The proof of the quadratic formula involves completing the square, see Section A.1. Starting from

$$ax^2 + bx + c = 0 \tag{A.2.3}$$

we immediately have

$$a\left(x + \frac{b}{2a}\right)^2 - \frac{b^2}{4a} + c = 0 \tag{A.2.4}$$

so that

$$\left(x + \frac{b}{2a}\right)^2 = \frac{b^2}{4a^2} - \frac{c}{a} \tag{A.2.5}$$

$$= \frac{b^2 - 4ac}{4a^2}. \tag{A.2.6}$$

Taking the square root of both sides and rearranging terms yields the quadratic formula in its standard form (A.2.2).

Definition A.2.2 Degeneracy. An nth-order polynomial always has n (complex) roots, but these roots may be repeated. In physics contexts, we call the physical quantity represented by the repeated root **degenerate**, see the contexts of matrix eigenvalues Section 4.2 and solutions of ODEs Section 15.6. A root that is repeated m times is called **m-fold degenerate**. ◊

A.3 Function Transformations

In pure mathematics settings, both the inputs and the outputs of functions are typically pure numbers, without dimensions, and the descriptions of functions like $\cos x$ and e^x are chosen to make them look as simple as possible. But, in applied settings these functions must be tailored to model the physical situation, by inserting parameters that may have dimensions, such as $A\cos(kx - \delta)$ and $Ae^{(kx-\delta)}$. How do these parameters change the shape of the graphs?

Activity A.3.1 Visualizing Parameters that Transform Functions. In the applet below, you can enter a function of your choice, of the form $Af(kx-\delta)$, where A, k, and δ are three arbitrary real parameters. (The default function is $A\cos(kx - \delta)$.) Determine how (and why!) the three parameters change the function.

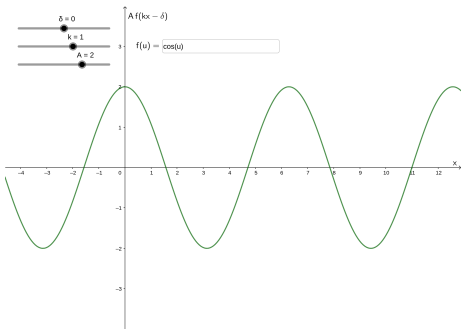


Figure A.3.1 An applet that allows you to change the values of A, k, and δ in $Af(kx - \delta)$. The default function displayed is $A\cos(kx - \delta)$.

Solution. Because A multiplies the overall value of the function (i.e. the range), increasing A increases the vertical extent of the graph by a factor of A. Because k multiplies the argument of the function (i.e. the domain), increasing k means the argument will increase faster, so the shape of function will be compressed horizontally. Because δ is subtracted from the argument of the function (i.e. the domain), increasing delta makes the argument look less than it really is, so the whole graph moves horizontally, to the right.

Definition A.3.2 Amplitude, Wave Number, Angular Frequency, and Phase. In the function $Af(kx - \delta)$, the parameter A is called the **amplitude**; the parameter k is called the **wave number**; and the parameter δ is called the **phase**. If the variable in the function is time t, then the functional form is usually written $Af(\omega t - \delta)$, and the parameter ω is called the **angular frequency** rather than wave number. ◊

Appendix B

Formulas

B.1 Coordinate Systems

B.1.1 Cylindrical Coordinates

$$\begin{aligned} x &= s\cos\phi & s^2 &= x^2 + y^2 \\ y &= s\sin\phi & \tan\phi &= y/x \\ z &= z & z &= z \end{aligned}$$

$$\begin{aligned} 0 \le s < \infty \\ 0 \le \phi < 2\pi \\ -\infty < z < \infty \end{aligned}$$

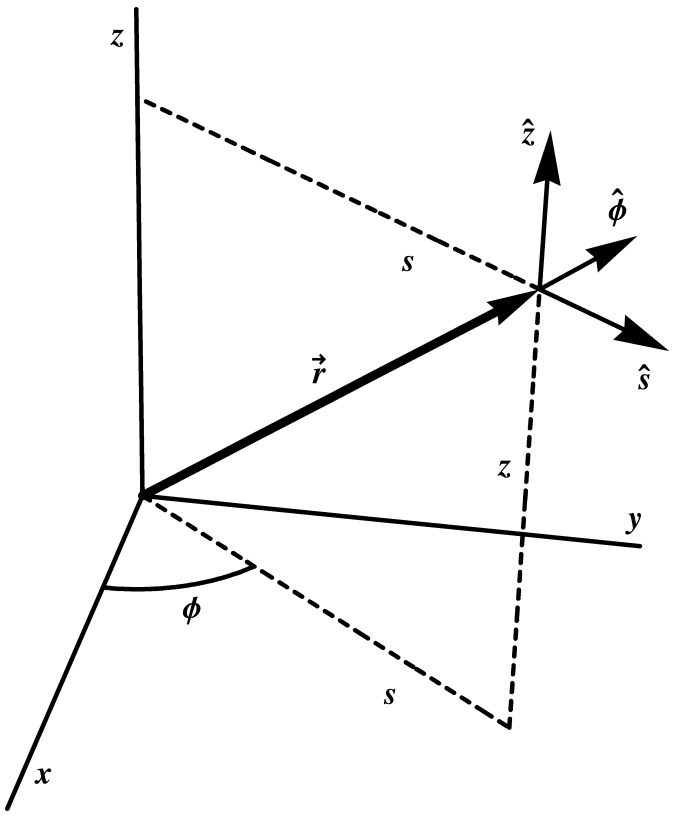


Figure B.1.1 The definition of cylindrical coordinates, also showing the associated basis vectors.

B.1.2 Spherical Coordinates

$$\begin{aligned} x &= r\sin\theta\cos\phi & r^2 &= x^2+y^2+z^2 \\ y &= r\sin\theta\sin\phi & \tan\theta &= \sqrt{x^2+y^2}/z \\ z &= r\cos\theta & \tan\phi &= y/x \end{aligned} \tag{B.1.1}$$

Be careful to remember the ranges of the two angles!

$$\begin{aligned} 0 &\le r < \infty \\ 0 &\le \theta < \pi \\ 0 &\le \phi < 2\pi \end{aligned}$$

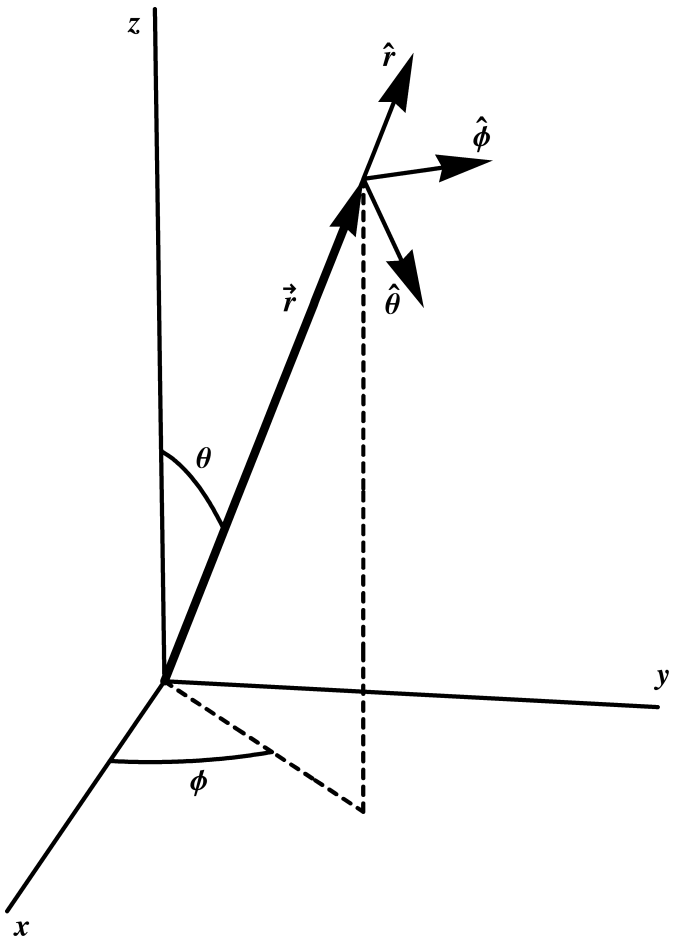


Figure B.1.2 The geometric definition of spherical coordinates, also showing the associated basis vectors.

Notation. Both of these coordinate systems reduce to polar coordinates in the x, y-plane, where $z = 0$ and $\theta = \pi/2$ if, in the cylindrical case you relabel s to the more standard r. In both cases, ϕ rather than θ is the label for the angle around the z-axis. Make sure you know which geometric angles θ and ϕ represent, rather than just memorizing their names. Whether or not you adopt the conventions used here, you should be aware that many different labels are in common use for both of these angles. In particular, you will often see the roles of θ and ϕ interchanged, particularly in mathematics texts.

Another common convention for curvilinear coordinates is to use ρ for the spherical coordinate r. We will not use ρ for the radial coordinate in spherical coordinates because we want to reserve it to represent charge or mass density. Some sources use r for both the axial distance in cylindrical coordinates and the radial distance in spherical coordinates.

B.2 Formulas for Div, Grad, Curl

B.2.1 Rectangular Coordinates

$$d\vec{\boldsymbol{r}} = dx\,\hat{\boldsymbol{x}} + dy\,\hat{\boldsymbol{y}} + dz\,\hat{\boldsymbol{z}}$$

$$\vec{\boldsymbol{F}} = F_x\,\hat{\boldsymbol{x}} + F_y\,\hat{\boldsymbol{y}} + F_z\,\hat{\boldsymbol{z}}$$

$$\begin{aligned}
\vec{\boldsymbol{\nabla}} f &= \frac{\partial f}{\partial x}\,\hat{\boldsymbol{x}} + \frac{\partial f}{\partial y}\,\hat{\boldsymbol{y}} + \frac{\partial f}{\partial z}\,\hat{\boldsymbol{z}} \\
\vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{F}} &= \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} \\
\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{F}} &= \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z}\right)\hat{\boldsymbol{x}} + \left(\frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x}\right)\hat{\boldsymbol{y}} + \left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y}\right)\hat{\boldsymbol{z}} \\
\nabla^2 f &= \frac{\partial^2 f}{dx^2} + \frac{\partial^2 f}{dy^2} + \frac{\partial^2 f}{dz^2}
\end{aligned}$$

B.2.2 Cylindrical Coordinates

$$\begin{aligned}
d\vec{\boldsymbol{r}} &= ds\,\hat{\boldsymbol{s}} + s\,d\phi\,\hat{\boldsymbol{\phi}} + dz\,\hat{\boldsymbol{z}} \\
\vec{\boldsymbol{F}} &= F_s\,\hat{\boldsymbol{s}} + F_\phi\,\hat{\boldsymbol{\phi}} + F_z\,\hat{\boldsymbol{z}}
\end{aligned}$$

$$\begin{aligned}
\vec{\boldsymbol{\nabla}} f &= \frac{\partial f}{\partial s}\,\hat{\boldsymbol{s}} + \frac{1}{s}\frac{\partial f}{\partial \phi}\,\hat{\boldsymbol{\phi}} + \frac{\partial f}{\partial z}\,\hat{\boldsymbol{z}} \\
\vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{F}} &= \frac{1}{s}\frac{\partial}{\partial s}\left(sF_s\right) + \frac{1}{s}\frac{\partial F_\phi}{\partial \phi} + \frac{\partial F_z}{\partial z} \\
\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{F}} &= \left(\frac{1}{s}\frac{\partial F_z}{\partial \phi} - \frac{\partial F_\phi}{\partial z}\right)\hat{\boldsymbol{s}} + \left(\frac{\partial F_s}{\partial z} - \frac{\partial F_z}{\partial s}\right)\hat{\boldsymbol{\phi}} + \frac{1}{s}\left(\frac{\partial}{\partial s}\left(sF_\phi\right) - \frac{\partial F_s}{\partial \phi}\right)\hat{\boldsymbol{z}} \\
\nabla^2 f &= \frac{1}{s}\frac{\partial}{\partial s}\left(s\frac{\partial f}{\partial s}\right) + \frac{1}{s^2}\frac{\partial^2 f}{d\phi^2} + \frac{\partial^2 f}{dz^2}
\end{aligned}$$

B.2.3 Spherical Coordinates

$$\begin{aligned}
d\vec{\boldsymbol{r}} &= dr\,\hat{\boldsymbol{r}} + r\,d\theta\,\hat{\boldsymbol{\theta}} + r\,\sin\theta\,d\phi\,\hat{\boldsymbol{\phi}} \\
\vec{\boldsymbol{F}} &= F_r\,\hat{\boldsymbol{r}} + F_\theta\,\hat{\boldsymbol{\theta}} + F_\phi\,\hat{\boldsymbol{\phi}}
\end{aligned}$$

$$\begin{aligned}
\vec{\boldsymbol{\nabla}} f &= \frac{\partial f}{\partial r}\,\hat{\boldsymbol{r}} + \frac{1}{r}\frac{\partial f}{\partial \theta}\,\hat{\boldsymbol{\theta}} + \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\,\hat{\boldsymbol{\phi}} \\
\vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{F}} &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 F_r\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta F_\theta\right) + \frac{1}{r\sin\theta}\frac{\partial F_\phi}{\partial \phi} \\
\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{F}} &= \frac{1}{r\sin\theta}\left(\frac{\partial}{\partial \theta}\left(\sin\theta F_\phi\right) - \frac{\partial F_\theta}{\partial \phi}\right)\hat{\boldsymbol{r}} + \frac{1}{r}\left(\frac{1}{\sin\theta}\frac{\partial F_r}{\partial \phi} - \frac{\partial}{\partial r}\left(rF_\phi\right)\right)\hat{\boldsymbol{\theta}} \\
&\quad + \frac{1}{r}\left(\frac{\partial}{\partial r}\left(rF_\theta\right) - \frac{\partial F_r}{\partial \theta}\right)\hat{\boldsymbol{\phi}} \\
\nabla^2 f &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial \phi^2}
\end{aligned}$$

Appendix C

Symbols

Symbol	Description	Page
$z = x + iy$	the rectangular form of a complex number z with real part x and imaginary part y	34
$\operatorname{Re} z$, $\Re z$	the real part of a complex number z or the real axis in the complex plane	34
$\operatorname{Im} z$, $\Im z$	the imaginary part of a complex number z or the imaginary axis in the complex plane	34
z^*, $\bar{z}$	complex conjugate of a complex number z	36
$\lvert z \rvert$	norm of a complex number z	37
$z = re^{i\phi}$	the exponential form of a complex number z	40
M^T	transpose of a matrix M	47
$A\lvert v\rangle = \lambda\lvert v\rangle$	the eigenvalue/eigenvector equation for a linear operator A	52
$[M, N] \equiv MN - NM$	the commutator of two operators M and N	57
$N^\dagger = N^{*T}$	the Hermitian conjugate (or adjoint) of a matrix N A	57
$P_v^2 = P_v$	the definition of a projection operator P_v	61
$P_v = \lvert v\rangle\langle v\rvert$	the bra-ket form of a projection operator P_v	61
$\{\sigma_x, \sigma_y, \sigma_z\}$	Pauli matrices	64
$\frac{dy}{dx}$	Leibniz notation for derivative	69
y'	Lagrange notation for derivative (w.r.t. x)	69
$\dot{y}$	Newton notation for derivative (w.r.t. t)	69
$\forall$	"for all"	145
$\langle\vec{u}\lvert\vec{v}\rangle$	the inner product of the vectors $\lvert\vec{u}\rangle$ and $\lvert\vec{v}\rangle$	151
ODE	ordinary differential equation	159
PDE	partial differential equation	159
$\mathcal{L}$	linear differential operator	160
$P_\ell(z)$	Legendre polynomial of degree ℓ	175
δ_{ij}	the Kronecker Delta	177
$\Theta(x)$	the step function (alternatively, theta or Heaviside function)	179
$\delta(x)$	the Dirac delta function (alternatively, distribution)	180

Appendix D

Notation

Appendix E

Definitions

(Continued on next page)

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An relatively easy to read Mathematical Methods text with many worked examples. Covers more content than our text at about the same level.

[**4**] George B. Arfken, and Hans J. Weber, *Mathematical Methods for Physicists*, 4th Edition, Academic Press, 1995.
An relatively easy to read Mathematical Methods text with many worked examples. Covers more content than our text at a somewhat higher level.

[**5**] K. F. Riley, M. P. Hobson, and S. J. Bence, *Mathematical Methods for Physics and Engineering*, 3rd Edition, Cambridge, 2006.
An harder to read Mathematical Methods text. Worked examples skip many steps. Covers tons of content at a much higher level than this text. A great graduate/professional resource.

[**6**] David J. Griffiths, *Introduction to Electrodynamics*, 4th Edition, Pearson, 2013.
THE standard upper-level undergraduate text on electromagnetism. Easy to read. Many worked examples. The vector calculus portion of our text is mainly an expansion of Chapters 1–3 and 5 of Griffiths.

[**7**] H. M. Schey *Div, Grad, Curl, and All That*, 4th edition, Norton, 2005.
Excellent informal introduction to the geometry of vector calculus.

Sections from Other Books

The sections below are referenced in this book, but appear in our other books. Just click on the link to be taken to the relevant section.

[1] https://books.physics.oregonstate.edu/GVC/polarint.html

[2] https://books.physics.oregonstate.edu/GSF/path.html

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