

## 7 INTEGRATION IN ONE AND MANY DIMENSIONS

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### 7.1 Integrating functions of one variable

A FOUNDATION IDEA IN CALCULUS is the concept of integration. The integral measures the area under the curve defined by the variation in a function over a range of its variable. In modeling physical processes, we are often interested in summing the value of one property (the given function) times the incremental change in another property (the variable). Pressure-volume work done by a gas is calculated by summing the pressure (the function) times the incremental change in volume (the variable) as the volume is varied. The computed pressure-volume work is the area under the pressure curve over a range of volume. In this section, we explore the definition of the integral and review the most commonly applied methods of integrating a function of one variable.

#### 7.1.1 The concept of the antiderivative and definition of the integral

We can think of an integral as an *antiderivative*. While differentiation is an operation that transforms a function into its derivative, integration is an operation that transforms the derivative of a function back to the original function. Consider the derivative of a function  $f(x)$  with respect to the variable  $x$  defined

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

Rearranging this result, we find an expression for the total differential:

$$df(x) = f'(x)dx$$

This expression relates the change in the function  $f(x)$  resulting from an incremental change in the variable  $dx$ . We can then define the *integral* as the operation that transforms the incremental change  $df(x)$  into the function  $f(x)$  itself:

$$f(x) = \int df(x) = \int f'(x)dx \quad (7.1)$$

The integral is the antiderivative because it transforms the derivative of a function into the function itself.

We developed a good working knowledge of differentiation in Chapter 3. That means we already know something about integrals as antiderivatives. For example, for  $x$  raised to a power  $n$ , we know that

$$f(x) = \frac{1}{n}x^n \Rightarrow f'(x) = x^{n-1}$$

which implies that<sup>1</sup>

$$\int f'(x)dx = \int x^{n-1} dx = \frac{1}{n}x^n = f(x)$$

Similarly, for the exponential function, we know that

$$f(x) = \frac{1}{a} e^{ax} \Rightarrow f'(x) = e^{ax}$$

so that

$$f(x) = \int f'(x)dx = \int e^{ax} dx = \frac{1}{a} e^{ax}$$

For the natural logarithm, we find

$$f(x) = \ln(x) \Rightarrow f'(x) = \frac{1}{x}$$

so that

$$f(x) = \int f'(x)dx = \int \frac{1}{x} dx = \ln(x)$$

Finally, for the sine and cosine functions, we find

$$f(x) = -\frac{1}{a} \cos(ax) \Rightarrow f'(x) = \sin(ax)$$

so that

$$f(x) = \int f'(x)dx = \int \sin(ax) dx = -\frac{1}{a} \cos(ax)$$

and

$$f(x) = \frac{1}{a} \sin(ax) \Rightarrow f'(x) = \cos(ax)$$

so that

$$f(x) = \int f'(x)dx = \int \cos(ax) dx = \frac{1}{a} \sin(ax)$$

Thinking of integration as antidifferentiation, our knowledge of differentiation immediately translates into a knowledge of integration. Taking any total derivative relation, we have a relation for an indefinite integral.

### 7.1.2 Interpretation of the integral

The derivative is interpreted as the rate of change in a function for a given value of its variable. The integral sign  $\int$  is an elongated S standing for summation. The process of integration is the process of summing the area under the curve of the function being integrated.<sup>2</sup>

Let's explore the interpretation of the integral through the example of determining the pressure-volume work done by an ideal gas at constant temperature, defined

$$w = \int_{V_A}^{V_B} p(V)dV = \int_{V_A}^{V_B} \frac{nRT}{V} dV$$

where we have used the ideal gas equation of state  $pV = nRT$  to define  $p(V) = \frac{nRT}{V}$ .<sup>3</sup> The function to be integrated, in this case  $p(V)$ , is known as the *integrand*. The factor  $nRT$  is a constant independent of  $V$  and can be pulled

<sup>1</sup> This form of integral, for which the range of  $x$  is unspecified, is known as an *indefinite integral*.

<sup>2</sup> The fact that the definite integral of a function over an interval is equal to the difference between the antiderivatives of the function evaluated at the endpoints of the interval is known as the *fundamental theorem of calculus*. The theorem was first presented by Scottish mathematician and astronomer *James Gregory* (1638-1675) and English theologian and mathematician *Isaac Barrow* (1630-1677). The theorem was built upon by Barrow's student *Isaac Newton* (1642-1727) and systematized by *Gottfried Leibniz* (1646-1716) who introduced the notation commonly used today.

<sup>3</sup> This form of integral, for which the range of  $x$  is specified, is known as a *definite integral*.

out of the integral, leaving

$$w = nRT \int_{V_A}^{V_B} \frac{1}{V} dV$$

From our antiderivative relations in the previous section, we know that

$$\int \frac{1}{x} dx = \ln(x)$$

so that<sup>4</sup>

$$w = nRT \int_{V_A}^{V_B} \frac{1}{V} dV = nRT \ln(V) \Big|_{V_A}^{V_B} = nRT \ln \left( \frac{V_B}{V_A} \right)$$

where we have used the fact that  $\ln(V_B) - \ln(V_A) = \ln \left( \frac{V_B}{V_A} \right)$ .

What is the physical interpretation of this result? We interpret the integral as the antiderivative. As such, the integral represents the summing up of many small changes in the work  $dw = p(V)dV$  that take place over many small changes in volume

$$w = \int dw = \int p(V) dV$$

Each increment of the work  $dw$  is the area formed by the height of the function  $p(V)$  times the width resulting from a change in volume  $dV$ .

Figure 7.1 shows  $p(V)$  as a function of volume  $V$  between the volumes  $V_A$  and  $V_B$ . Suppose we divide the interval  $[V_A, V_B]$  into  $N$  subintervals  $[V_1, V_2], [V_2, V_3], \dots, [V_N, V_{N+1}]$  where  $V_1 = V_A, V_{N+1} = V_B$  and  $V_n = V_A + (n - 1)\Delta V$ . The width of each interval is  $\Delta V = (V_B - V_A)/N$ . We can approximate the integral defined as the area under the curve using the sum

$$\begin{aligned} w &\approx p(V_1)\Delta V + p(V_2)\Delta V + \dots + p(V_N)\Delta V \\ &= \sum_{n=1}^N p(V_n)\Delta V \end{aligned}$$

which is the sum of the areas of  $N$  rectangles each of width  $\Delta V$  and height  $p(V_n)$ . Each shaded area is an increment of work  $dw$ . The integral is the sum of many of these areas adding up to the total change  $w$ .

As  $N$  increases, the number of rectangles increases and the accuracy of the estimate to the area under the curve improves. In the limit  $N \rightarrow \infty$ , the sum converges to the exact result

$$w = \lim_{N \rightarrow \infty} \sum_{n=1}^N p(V_n)\Delta V = \int_{V_A}^{V_B} p(V)dV \quad (7.2)$$

The area under the curve between the lower limit of integration  $V_A$  and the upper limit of integration  $V_B$  represents the definite integral of  $p(V)$  taken between  $V_A$  and  $V_B$ .

Our choice of the height of each rectangle as the leftmost point in the interval was arbitrary. We could just as well take the rightmost point in the

<sup>4</sup> Note that  $f(x) \Big|_{x_1}^{x_2} = f(x_2) - f(x_1)$ .

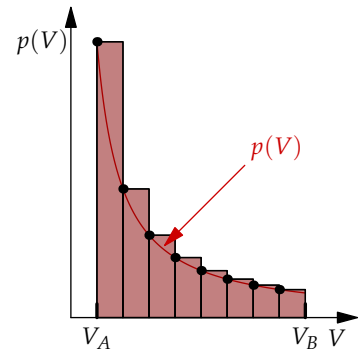


Figure 7.1: The integral of  $p(V)$  between  $V_A$  and  $V_B$  is the area under the curve. The integral can be approximated by the sum of the shaded rectangular areas

$$\sum_{n=1}^N p(V_n)\Delta V$$

where  $V_n = V_A + (n - 1)\Delta V$ . For finite  $\Delta V$  this approximation overestimates the exact integral.

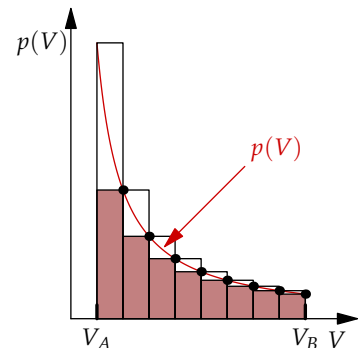


Figure 7.2: Alternatively, the integral can be approximated by the sum of the shaded rectangular areas  $p(V_n)\Delta V$  where  $V_n = V_A + n\Delta V$ . For finite  $\Delta V$  this approximation underestimates the exact integral.

interval to be the height of the rectangle. In that case, the sum approximating the integral is

$$w = \lim_{N \rightarrow \infty} \sum_{n=1}^N p(V_{n+1})\Delta V = \int_{V_A}^{V_B} p(V)dV \quad (7.3)$$

which represents the shaded area in Figure 7.2. Note that for finite  $\Delta V > 0$ , the first approximation using the leftmost point in the interval leads to an overestimate of the area under the curve. In contrast, using the rightmost point in the interval leads to an underestimate of the area under the curve. Nevertheless, in the limit  $\Delta V \rightarrow 0$  both approximations lead to the same exact result.

With these insights, we can develop a general definition of the integral in terms of the *Riemann sum*. Suppose we partition the interval  $[V_A, V_B]$  into  $N$  subintervals  $[V_1, V_2], [V_2, V_3], \dots, [V_N, V_{N+1}]$  where  $V_A = V_1 < V_2 < \dots < V_N < V_{N+1} = V_B$ . The integral of  $p(V)$  between  $V_A$  and  $V_B$  can be approximated by the sum

$$w = \lim_{N \rightarrow \infty} \sum_{n=1}^N p(V_n^*)\Delta V_n = \int_{V_A}^{V_B} p(V)dV \quad (7.4)$$

where  $V_n^* \in [V_n, V_{n+1}]$  and  $\Delta V_n = V_{n+1} - V_n$ . An example of a Riemann sum having subintervals of varying width  $\Delta V_n$  and randomly chosen points  $V_n^*$  within each subinterval is shown in Figure 7.3.

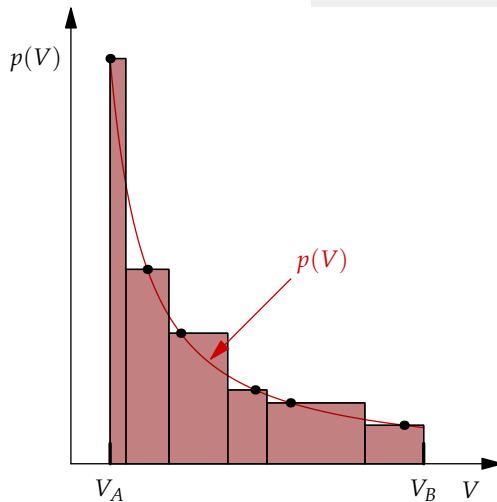


Figure 7.3: The integral of  $p(V)$  between  $V_A$  and  $V_B$  can be approximated by the Riemann sum

$$\sum_{n=1}^N p(V_n^*)\Delta V_n$$

where  $V_n^* \in [V_n, V_{n+1}]$  and  $\Delta V_n = V_{n+1} - V_n$ . As  $N \rightarrow \infty$  the sum converges to the exact result.

In our previous sums, the subintervals  $\Delta V_n$  were of uniform width. In this Riemann sum, the intervals  $V_n$  may be of varying width. Moreover, in our previous sums the height of each rectangle was taken to be the value of  $p(V)$  for the leftmost or rightmost point in the interval. In the Riemann sum, the height of the rectangle is taken to be  $p(V_n^*)$  where  $V_n^*$  is any point in the interval  $[V_n, V_{n+1}]$ .<sup>5</sup>

<sup>5</sup> The results in Equations 7.2 and 7.3 are known as *left method* and *right method* Riemann sums, respectively. Alternative definitions include the *maximum method* and *minimum method* for which the height of each rectangle is defined by the endpoint with the larger or smaller value, respectively.

We can now combine our definition of the derivative given by Equation 3.2

$$\lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} = \frac{df}{dx}$$

with our equivalent definition of the integral

$$\lim_{N \rightarrow \infty} \sum_{n=1}^N f(x_n) \Delta x = \int f(x) dx \tag{7.5}$$

These geometric interpretations of the derivative and integral in terms of *finite differences*  $\Delta x$  in the variable  $x$  are useful in numerically estimating derivatives and integrals when the indefinite integrals or exact derivatives are not known. By performing the sum for increasing values of  $N$  and decreasing values of  $\Delta x$ , we find an increasingly accurate approximation of the integral.

### 7.1.3 Revisiting the rules for integrating functions of one variable

There are a number of useful rules for integrating functions of one variable. We introduce these rules by exploring the integration of a variety of commonly appearing functional forms. It is important to practice and master these rules. They are essential to our successful application of calculus to problems in the physical sciences.

1.  $df(x)$ . Integration of the exact differential of a function leads to the function itself plus an *integration constant*<sup>6</sup> written  $C$ :

$$\int df(x) = f(x) + C \tag{7.6}$$

For example, suppose  $df(x) = dx$ , then

$$\int df(x) = \int dx = x + C$$

In evaluating indefinite integrals, it is important to remember to include the integration constant  $C$ .

2.  $a$ . Integration of a constant produces a linear function plus an integration constant:

$$\int a dx = a \int dx = ax + C \tag{7.7}$$

Differentiation of the result produces  $a$ . Note that when we have a constant times a function of  $x$ , we can pull the constant out of the integral as shown above. Pulling the constant out in front of the integral can be helpful in simplifying the integration of complicated expressions.

3.  $x^n$ . Using our knowledge of the *power rule* for derivatives of powers of  $x$ , we find

$$\int x^n dx = \frac{1}{n+1} x^{n+1} + C \quad n \neq -1 \tag{7.8}$$

Let's use this result to evaluate the integral

$$\int v_0 t dt$$

<sup>6</sup> The derivative of a function is equal to the derivative of the same function plus a constant

$$\frac{d}{dx} f(x) = \frac{d}{dx} (f(x) + C)$$

As such, the antiderivative of a function equals the integral of that function plus a constant

$$\int df(x) = f(x) + C$$

The *integration constant*  $C$  is undetermined for an indefinite integral. It can be evaluated once the limits of integration are defined.

We find

$$\int v_0 t dt = v_0 \int t dt = \frac{1}{2} v_0 t^2 + C$$

Further consider the integral

$$\int \frac{\Delta H}{RT^2} dT$$

Using our result we find

$$\int \frac{\Delta H}{RT^2} dT = \frac{\Delta H}{R} \int \frac{1}{T^2} dT = -\frac{\Delta H}{R} \frac{1}{T} + C$$

Differential and integral relations of this kind are commonly encountered in thermodynamics.

4.  $x^{-1}$ . Using our knowledge of the derivative of the natural logarithm, we find the indefinite integral

$$\int \frac{1}{x} dx = \ln x + C \tag{7.9}$$

The definite integral of  $\frac{1}{x}$  over the range  $x \in [a, b]$  can be written

$$\int_a^b \frac{1}{x} dx = \ln x \Big|_a^b = \ln(b) - \ln(a) = \ln\left(\frac{b}{a}\right)$$

This result is shown graphically in Figure 7.4. The integral is equal to the shaded area under the curve. The black line shows the accumulating area under the curve, which increases according to  $\ln\left(\frac{x}{a}\right)$ .

In the kinetics of certain reactions, the rate of change in the concentration  $c(t)$  is proportional to the concentration itself. As the rate of change in  $c(t)$  is  $dc/dt$ , this proportional relationship can be written

$$\frac{dc}{dt} = -kc \tag{7.10}$$

By separating  $dc$  from  $dt$  and dividing each side by  $c$ , this equation can be reformed as

$$\frac{1}{c} dc = -k dt$$

where  $k$  is a constant.<sup>7</sup> We can solve this equation for  $c(t)$ . Using our knowledge of integrals, we can transform the result

$$\int \frac{1}{c} dc = - \int k dt$$

into a relation for the concentration as a function of time

$$\ln c(t) = -kt + C$$

By exponentiating each side of this equation, the result can also be expressed as

$$c(t) = Ae^{-kt}$$

where  $A = e^C$ .

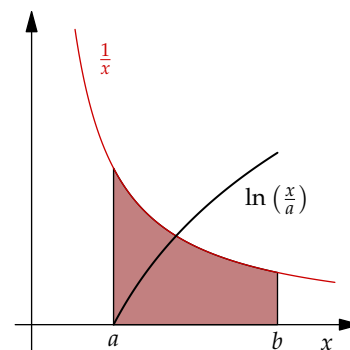


Figure 7.4: The function  $\frac{1}{x}$  over a range of  $x$  (red line). The integral of  $\frac{1}{x}$  between  $x = a$  and  $x = b$  is the shaded area under the curve. The accumulating area under the curve  $\ln\left(\frac{x}{a}\right)$  (black line) is 0 at  $x = a$  and grows to the final value of the integral  $\ln\left(\frac{b}{a}\right)$  at  $x = b$ .

<sup>7</sup> Here we treat the derivative  $\frac{dc}{dt}$  as a fraction, which allows us to separate the incremental change in concentration,  $dc$ , from the incremental change in time,  $dt$ .

As another example, consider the following fundamental relation<sup>8</sup> in thermodynamics:

$$\frac{dp}{dT} = \frac{\Delta H}{RT^2} p \tag{7.11}$$

By separating  $dp$  from  $dT$  and dividing each side by  $p$ , this equation can be reformed as

$$\frac{1}{p} dp = \frac{\Delta H}{RT^2} dT$$

We solve the latter equation for  $p(T)$  using our knowledge of integrals as

$$\int \frac{1}{p} dp = \frac{\Delta H}{R} \int \frac{1}{T^2} dT$$

and

$$\ln p = -\frac{\Delta H}{RT} + C$$

This can be rewritten in the familiar form

$$p(T) = A \exp\left(-\frac{\Delta H}{RT}\right)$$

where  $\ln A = C$ . Inserting our result in Equation 7.11 demonstrates the validity of our solution.

<sup>8</sup> Known as the *Clausius-Clapeyron equation*, this relation describes the dependence of the vapor pressure on temperature. Note that we treat  $\frac{dp}{dT}$  as an algebraic ratio, which allows us to separate the incremental changes  $dp$  and  $dT$ .

5.  $f(x) + g(x)$ . Integration is a linear operation, like multiplication or differentiation. The integral of the sum of two functions is the sum of two integrals:

$$\int [f(x) + g(x)] dx = \int f(x) dx + \int g(x) dx \tag{7.12}$$

For example, consider the integral of the function  $C_p(T) = a + bT + cT^2$  over  $T$ , where  $a$ ,  $b$ , and  $c$  are constants. We find

$$\begin{aligned} \int C_p(T) dT &= \int (a + bT + cT^2) dT = a \int dT + b \int T dT + c \int T^2 dT \\ &= aT + \frac{1}{2}bT^2 + \frac{1}{3}bT^3 + C \end{aligned}$$

The integration of each term in  $C_p(T)$  increases the power of  $T$ . As we are taking an indefinite integral, it is important to include the integration constant  $C$  in our final result.

6.  $e^{ax}$ . Using our knowledge of the derivative of the exponential function, we find

$$\int e^{ax} dx = \frac{1}{a} e^{ax} + C \tag{7.13}$$

For example, consider the indefinite integral over a function  $c(t)$  with respect to  $t$ , where  $c(t) = C_0 e^{-t/\tau}$  and  $C_0$  and  $\tau$  are constants. We find

$$\int C_0 e^{-t/\tau} dt = C_0 \int e^{-t/\tau} dt = -C_0 \tau e^{-t/\tau} + C$$

Further consider the definite integral of  $e^{-x}$  over the range  $x \in [a, b]$ . We

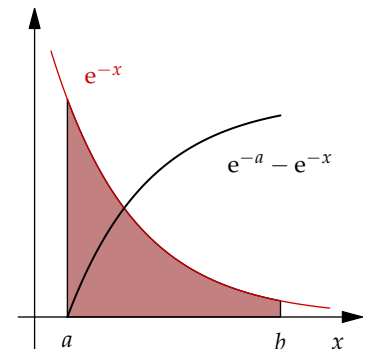


Figure 7.5: The function  $e^{-x}$  over a range of  $x$  (red line). The integral of  $e^{-x}$  between  $x = a$  and  $x = b$  is the shaded area under the curve. The accumulating area under the curve  $e^{-a} - e^{-x}$  (black line) is 0 at  $x = a$  and grows to the final value of the integral ( $e^{-a} - e^{-b}$ ) at  $x = b$ .

find

$$\int_a^b e^{-x} dx = -e^{-x} \Big|_a^b = e^{-a} - e^{-b}$$

This result is shown graphically in Figure 7.5. The decaying exponential is commonly encountered in physical kinetics, where it is used to model a decreasing population of species.

7.  **$\sin(ax)$  and  $\cos(ax)$** . Using our knowledge of derivatives of sine and cosine functions, we find

$$\int \sin(ax) dx = -\frac{1}{a} \cos(ax) + C \tag{7.14}$$

$$\int \cos(ax) dx = \frac{1}{a} \sin(ax) + C \tag{7.15}$$

For example, consider the integral over a sinusoidal function

$$\int_0^\pi \sin(x) dx = -\cos(x) \Big|_0^\pi = \cos(0) - \cos(\pi) = 1 - (-1) = 2$$

This result is shown graphically in Figure 7.6.

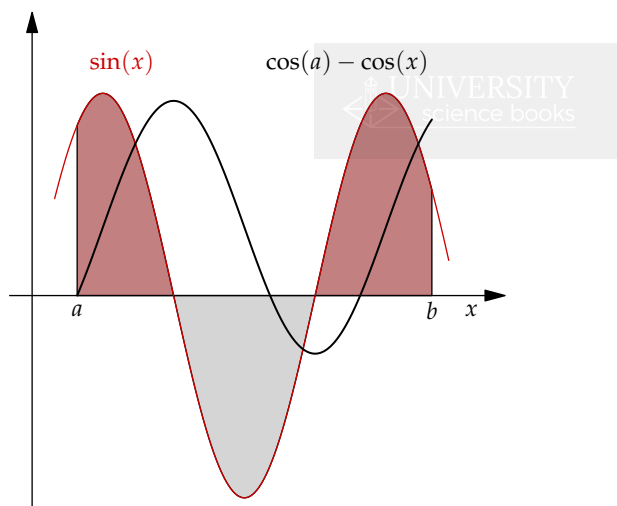


Figure 7.6: The function  $\sin(x)$  over a range of  $x$  (red line). The integral of  $\sin(x)$  between  $x = a$  and  $x = b$  has both positive (shaded red) and negative (shaded gray) contributions. The accumulating area under the curve  $\cos(a) - \cos(x)$  (black line) is 0 at  $x = a$  and grows to the final value of the integral  $(\cos(a) - \cos(b))$  at  $x = b$ .

The sinusoidal function takes on positive and negative values which add and subtract from the total area under the curve. The result is an accumulating area that oscillates as the contributions from positive and negative regions of the sine are summed.

8.  **$\delta(x - x_0)$** . The *Dirac delta function* (or  $\delta$  function) was discovered by Paul Dirac<sup>9</sup> and plays an important role in the mathematics of quantum mechanics. While the function may seem strange, in some ways, the integral over the  $\delta$  function could not be simpler. The function  $\delta(x - x_0)$  is zero everywhere except at the point  $x = x_0$ , where it is infinite:

$$\delta(x - x_0) = \begin{cases} \infty & x = x_0 \\ 0 & x \neq x_0 \end{cases} \tag{7.16}$$

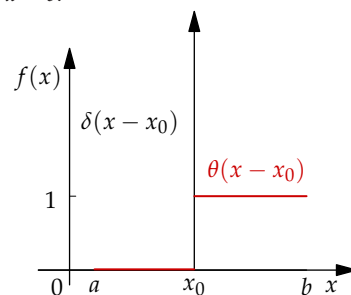


Figure 7.7: The function  $\delta(x - x_0)$  over a range of  $x$ , where the black arrow located at  $x = x_0$  is directed toward a single point at infinity. The integral of  $\delta(x - x_0)$  between  $x = a$  and  $x = b$  is the accumulating area under the curve (red line) represented by the *Heaviside step function*  $\theta(x - x_0)$ , which is 0 for  $x < x_0$  and unity for  $x \geq x_0$ .

<sup>9</sup> The English physicist *Paul Dirac* (1902-1984) made fundamental contributions to quantum theory.



The area under the function when integrated over a range of  $x$  containing  $x_0$  is unity, as

$$\int_{-\infty}^{\infty} \delta(x - x_0) dx = 1$$

An attempt to graphically depict the Dirac delta function is shown in Figure 7.7.<sup>10</sup>

Consider the integration over all space of the delta function multiplying a function  $f(x)$ . The product of  $f(x)\delta(x - x_0)$  is zero everywhere except at  $x = x_0$ , so that

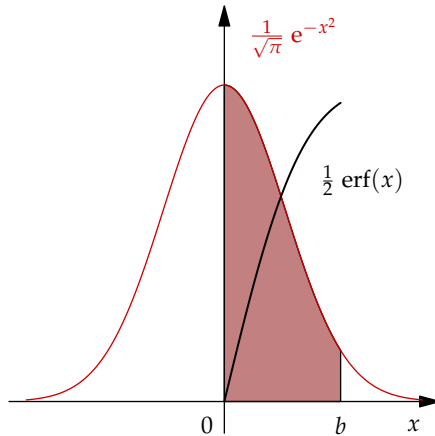
$$\int_{-\infty}^{\infty} f(x)\delta(x - x_0) dx = f(x_0) \int_{-\infty}^{\infty} \delta(x - x_0) dx = f(x_0)$$

Note that we can pull the term  $f(x_0)$  out of the integral as it is a constant. We will explore the utility of the delta function later in this chapter.

9.  $e^{-ax^2}$ . The gaussian function has many important applications in the physical sciences. There is a simple closed form solution for the definite integral of the gaussian function over all space:

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \tag{7.17}$$

This fundamentally important result is widely used in applications of integration in the physical sciences. The identity is proven in the complements.



<sup>10</sup>Note that as the Heaviside step function is related to the integral over the delta function as

$$\theta(x - x_0) = \int_{-\infty}^x \delta(x' - x_0) dx'$$

it follows that the derivative of the Heaviside step function

$$\frac{d\theta(x - x_0)}{dx} = \delta(x - x_0)$$

is the delta function.

Figure 7.8: The function  $\frac{1}{\sqrt{\pi}}e^{-x^2}$  over a range of  $x$  (red line). The integral of  $e^{-x^2}$  between  $x = 0$  and  $x = b$  is the shaded area under the curve. The accumulating area under the curve  $\frac{1}{2}\text{erf}(x)$  (black line) is zero at  $x = 0$  and grows to the final value  $\frac{1}{2}\text{erf}(b)$  at  $x = b$ .

The integral over a gaussian function occurs frequently in the physical sciences. It is called the *error function* and is defined

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \tag{7.18}$$

The error function is positive for positive values of  $x$ , representing the area under the gaussian function over the range  $[0, x]$  (see Figure 7.8). There is

also a *complementary error function* that is defined

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt = 1 - \operatorname{erf}(x) \quad (7.19)$$

and represents the area under the gaussian function not included in the error function. As such,  $\operatorname{erf}(x) + \operatorname{erfc}(x) = 1$  (see Figure 7.8). Numerical values of the error function and complementary error function are tabulated in Supplement S7.

The rules of integration above provide us with the foundation of knowledge we need to address problems in the physical sciences that involve the integration of functions.

### 7.1.4 Useful tricks for integrating functions of one variable

In addition to using the fundamental rules of integration previously introduced, we can add to our toolbox a few basic tricks that will prove useful in performing integrals on more complicated functions.

1. **Algebraic substitution.** In differentiation we encountered complicated expressions that were simplified using an *algebraic substitution* of variables. For example, consider the function

$$f(x) = e^{-\frac{1}{x}}$$

Taking the derivative of this function with respect to  $x$  can be simplified by introducing the variable

$$y = \frac{1}{x}$$

where

$$\frac{dy}{dx} = -\frac{1}{x^2}$$

Using the chain rule defined

$$\frac{df}{dx} = \frac{df}{dy} \frac{dy}{dx}$$

the derivative of  $f(x)$  with respect to  $x$  can be expressed as

$$\frac{d}{dx} \left( e^{-\frac{1}{x}} \right) = \frac{d}{dy} e^{-y} \frac{dy}{dx} = -e^{-y} \left( -\frac{1}{x^2} \right) = \frac{1}{x^2} e^{-1/x}$$

We can use a similar trick in integration. Suppose we want to integrate the function

$$f(x) = \frac{1}{x^2} e^{-\frac{1}{x}}$$

This looks hard! We first simplify the function with the substitution<sup>11</sup>

$$y = \frac{1}{x} \quad dy = -\frac{1}{x^2} dx$$

This allows us to write

$$\int \frac{1}{x^2} e^{-\frac{1}{x}} dx = - \int e^{-y} dy = e^{-y} + C = e^{-\frac{1}{x}} + C$$

<sup>11</sup> Using the fact that

$$\frac{dy}{dx} = -\frac{1}{x^2}$$

we multiply both sides of the expression by  $dx$  to find

$$dy = -\frac{1}{x^2} dx$$

where as a final step we convert back to the original variable  $x$ . This example demonstrates how a clever substitution of variables turns an apparently challenging integral into a problem with a familiar solution.<sup>12</sup>

Further consider the example

$$\int \frac{1}{V - nb} dV \quad (7.20)$$

We make the algebraic substitution commonly referred to as  $u$ -substitution

$$u = V - nb \quad \frac{du}{dV} = 1 \quad du = dV$$

Inserting these results in our integral, we find

$$\int \frac{1}{V - nb} dV = \int \frac{1}{u} du = \ln u + C = \ln(V - nb) + C$$

While the proper substitution may be apparent in this example, in other cases careful consideration and trial and error may be required to identify the optimal  $u$ -substitution.

Finally, consider the example

$$\int \cos^2 x \sin x dx$$

We make the algebraic substitution

$$u = \cos x \quad du = -\sin x dx$$

and find

$$\int \cos^2 x \sin x dx = -\int u^2 du = -\frac{1}{3}u^3 + C = -\frac{1}{3}\cos^3 x + C$$

A wide range of integrals can be solved using algebraic substitution, including integrals involving polynomial, exponential, and sinusoidal integrands. Algebraic substitution is particularly valuable in the physical sciences, as the proper substitution of variables can convert a complicated integrand into a simplified and manageable function.

2. **Trigonometric transformation.** Consider the integral

$$\int \sin^2 x dx$$

We know how to integrate  $\sin x$  but not  $\sin^2 x$ . Fortunately, we can get rid of the square by transforming the expression using the *trigonometric transformation*

$$\sin^2 x = \frac{1}{2}(1 - \cos(2x))$$

so that

$$\begin{aligned} \int \sin^2 x dx &= \int \frac{1}{2}(1 - \cos(2x)) dx = \frac{1}{2} \int dx - \frac{1}{2} \int \cos(2x) dx \\ &= \frac{1}{2}x - \frac{1}{4}\sin(2x) + C \end{aligned}$$

<sup>12</sup> Using this trick we can show that the integral

$$\int e^{-\frac{\Delta E}{k_B T}} \left( \frac{\Delta E}{k_B T^2} \right) dT$$

with the substitution of variables  $u = -\frac{\Delta E}{k_B T}$  is equal to

$$e^{-\frac{\Delta E}{k_B T}} + C$$



When you encounter an integral over a trigonometric function that you don't recognize, consider trigonometric identities that might transform the integral into a solvable form.

3. **Partial fractions.** For an integral like Equation 7.20, the numerator  $dx$  is a derivative of the denominator  $(V - nb)$ . In that case, the integral can be solved using *algebraic substitution*. However, for the integral

$$\int \frac{1}{(a-x)(b-x)} dx$$

the numerator  $dx$  is not the derivative of the denominator  $(a-x)(b-x)$ . In this case, we can reform our integral using *partial fractions*.<sup>13</sup>

We can make use of a clever identity relating the product of the reciprocal differences to the difference of the reciprocal differences.<sup>14</sup> It is written as

$$\frac{1}{(a-x)(b-x)} = \frac{1}{(b-a)} \left( \frac{1}{a-x} - \frac{1}{b-x} \right)$$

and leads to the equality

$$\int \frac{1}{(a-x)(b-x)} dx = \int \frac{1}{(b-a)} \left( \frac{1}{a-x} - \frac{1}{b-x} \right) dx$$

As such, we can evaluate these integrals using our knowledge of the integral identity

$$\int \frac{1}{(x+a)} dx = \ln(x+a) + C$$

It follows that

$$\int \frac{1}{(b-a)} \left( \frac{1}{a-x} \right) dx = -\frac{1}{b-a} \ln(a-x) + C$$

and

$$\int \frac{1}{(b-a)} \left( \frac{1}{b-x} \right) dx = -\frac{1}{b-a} \ln(b-x) + C$$

resulting in

$$\int \frac{1}{(a-x)(b-x)} dx = \frac{1}{b-a} \ln \left( \frac{b-x}{a-x} \right) + C$$

The transformation of  $\frac{1}{(a-x)(b-x)}$  using partial fractions is graphically depicted in Figure 7.9. It is somewhat remarkable that the product of the reciprocal functions  $(a-x)^{-1}$  and  $(b-x)^{-1}$  is proportional to the difference of the two functions.

4. **Integration by parts.** A final trick for evaluating integrals found in the physical sciences is known as *integration by parts*. Recall the *product rule*

$$\frac{d}{dx} [u(x)v(x)] = u(x) \frac{dv}{dx} + v(x) \frac{du}{dx}$$

Multiplying both sides of the equation by  $dx$  results in

$$d(uv) = u dv + v du$$

<sup>13</sup> The method of partial fractions is a special case of the more general *Heaviside cover-up method* named for English physicist and engineer *Oliver Heaviside* (1850-1925).

<sup>14</sup> We can prove this

$$\begin{aligned} & \frac{1}{(b-a)} \left( \frac{1}{a-x} - \frac{1}{b-x} \right) \\ &= \frac{1}{(b-a)} \left[ \frac{b-x}{(a-x)(b-x)} - \frac{a-x}{(a-x)(b-x)} \right] \end{aligned}$$

that can be simplified as

$$\frac{1}{(b-a)} \left[ \frac{b-x-(a-x)}{(a-x)(b-x)} \right] = \frac{1}{(a-x)(b-x)}$$

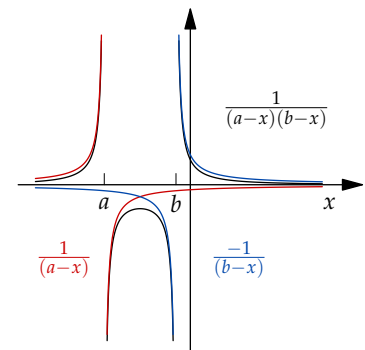


Figure 7.9: The function  $\frac{1}{(a-x)(b-x)}$  (black line) alongside the partial fractions  $\frac{1}{a-x}$  (red line) and  $\frac{-1}{b-x}$  (blue line) over a range of  $x$ .

which can be reformed as

$$udv = d(uv) - vdu$$

Integrating both sides of this equation leads to<sup>15</sup>

$$\int udv = uv - \int vdu \tag{7.21}$$

This relation expresses one integral  $\int udv$ , which may be challenging to evaluate, in terms of another integral  $\int vdu$ , which may be easier to solve, and a surface term  $uv$ , which is often zero. Equation 7.21 serves as our starting point for integration by parts.<sup>16</sup>

Let's see how this works. Consider the integral

$$\int_0^{\infty} xe^{-ax} dx = \int udv$$

We decompose  $xe^{-ax} dx = u dv$  as<sup>17</sup>

$$\begin{aligned} u &= x & dv &= e^{-ax} dx \\ du &= dx & v &= -\frac{1}{a}e^{-ax} \end{aligned} \tag{7.22}$$

Combining these results with Equation 7.21, we find<sup>18</sup>

$$\begin{aligned} \int_0^{\infty} xe^{-ax} dx &= \int udv = uv - \int vdu \\ &= -\frac{1}{a}xe^{-ax} \Big|_0^{\infty} - \int_0^{\infty} \left(-\frac{1}{a}e^{-ax}\right) dx = -\frac{1}{a^2}e^{-ax} \Big|_0^{\infty} = \frac{1}{a^2} \end{aligned}$$

As a final example of integration by parts, consider the indefinite integral

$$\int x \sin x dx = \int udv$$

We decompose  $x \sin x dx = u dv$  as

$$\begin{aligned} u &= x & dv &= \sin x dx \\ du &= dx & v &= -\cos x \end{aligned} \tag{7.23}$$

Combining these results with Equation 7.21, we find

$$\begin{aligned} \int x \sin x dx &= \int udv = uv - \int vdu \\ &= -x \cos x + \int \cos x dx \\ &= -x \cos x + \sin x dx + C \end{aligned}$$

where  $C$  is an undetermined integration constant.

This concludes our review of useful rules for integrating functions of one variable. In the physical sciences, we often encounter functions of many variables. In the next section, we apply the rules for integrating functions of one variable to the integration of functions of many variables.

<sup>15</sup> Integration by parts was first introduced by English mathematician Brook Taylor (1685-1731).

<sup>16</sup> We have used the identity

$$\int df(x) = f(x)$$

to write

$$\int d(uv) = uv$$

<sup>17</sup> To find  $v$  we integrate  $dv$  as

$$v = \int dv = \int e^{-ax} dx = -\frac{1}{a} e^{-ax}$$

while  $du$  is the total differential  $dx$ .

<sup>18</sup> We use the result

$$\frac{1}{a}xe^{-ax} \Big|_0^{\infty} = 0$$

At the lower limit  $xe^{-ax}$  is zero when  $x = 0$ . For the upper limit we find

$$\lim_{x \rightarrow \infty} xe^{-ax} = 0$$

This can be shown using l'Hôpital's rule as

$$\lim_{x \rightarrow \infty} \frac{x}{e^{ax}} = \lim_{x \rightarrow \infty} \frac{1}{ae^{ax}} = 0$$

## 7.2 Integrating functions of many variables

FUNCTIONS OF MORE THAN ONE VARIABLE are commonly encountered in modeling the properties of physical systems. The concentration of a substance in three-dimensions is a function of the position in space defined by the values of three cartesian coordinates. The total amount of substance in a given volume of solution is the multiple integral of the concentration taken over all three coordinates. In this section, we explore the definition of multiple integrals and survey common methods for evaluating multiple integrals over functions of many variables.

### 7.2.1 Double integrals

We represent the integral of a function of one variable  $f(x)$ , taken between points  $x = a$  and  $x = b$ , as

$$\int_a^b f(x) dx$$

We interpret this integral to be the area under the curve formed by  $f(x)$  over  $x \in [a, b]$ . An example is shown in Figure 7.10, where the shaded area is the value of the integral. This concept can be generalized to integrals of functions of many variables.

In two dimensions, we represent the *double integral* of a function  $f(x, y)$ , taken over a rectangular area on the  $xy$ -plane defined by  $x \in [a, b]$  and  $y \in [c, d]$ , as

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

We interpret this double integral to be the volume under the surface formed by  $f(x, y)$  over the rectangular area. An example is shown in Figure 7.11, where the shaded volume is the value of the integral.

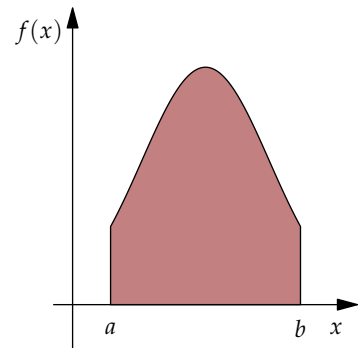


Figure 7.10: The function  $f(x)$  shown over a range of  $x$  from  $[a, b]$ . The integral  $\int_a^b f(x) dx$  equals the shaded area under the curve.

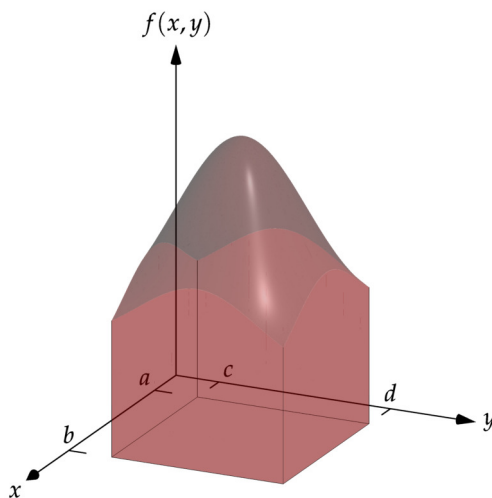


Figure 7.11: The function  $f(x, y)$  shown as a surface over a rectangular region on the  $xy$ -plane formed by  $x \in [a, b]$  and  $y \in [c, d]$ . The integral  $\int_c^d \int_a^b f(x, y) dx dy$  equals the shaded volume under the surface.

It is important to understand the notation used for a double integral. For a double integral, the order of integration is indicated by the order of the

increments  $dx$  and  $dy$  in the expression. Consider the integral

$$\int_c^d \int_a^b f(x, y) \, dx dy = \int_c^d \left[ \int_a^b f(x, y) \, dx \right] dy$$

Integration over  $x$  is performed first, followed by integration over  $y$ . Note that the *antiderivative* is defined strictly for functions of one variable (see Equation 7.1). As such, the definition of the *indefinite integral* does not immediately extend to functions of many variables.

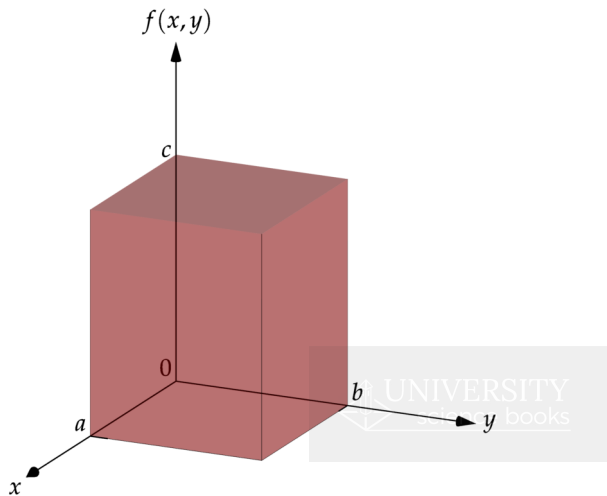


Figure 7.12: The function  $f(x, y) = c$  over a rectangular region on the  $xy$ -plane formed by  $x \in [0, a]$  and  $y \in [0, b]$ . The integral  $\int_0^b \int_0^a f(x, y) \, dx dy$  equals the shaded volume  $V = abc$ .

Let's consider a simple example to see how the double integral works. Suppose we wish to integrate the constant function  $f(x, y) = c$  over an area defined by  $x \in [0, a]$  and  $y \in [0, b]$  (see Figure 7.12). Since the function is a constant, we can write

$$\int_0^b \int_0^a f(x, y) \, dx dy = c \int_0^b \int_0^a \, dx dy$$

Since the limits of integration over  $x$  do not depend on  $y$ , we can separate the integral over  $x$  from the integral over  $y$  as

$$c \int_0^b \int_0^a \, dx dy = c \int_0^b \, dy \times \int_0^a \, dx$$

We have now reduced our two-dimensional integral to two one-dimensional integrals that we can readily evaluate to find

$$c \int_0^b \, dy \times \int_0^a \, dx = cb \int_0^a \, dx = cba$$

The value of the double integral is the height of the function,  $c$ , times the area over which the integral is performed on the  $xy$ -plane,  $ab$ , which is the volume  $abc$ .

### 7.2.2 Double integrals and the order of integration

Not all integrals on the  $xy$ -plane are as simple as our previous example. Consider the challenge of finding the area between a straight line and intersecting parabola shown in Figure 7.13. We define the area as the double integral over the  $xy$ -plane restricted to the area between the curves.

Suppose we wish to first integrate over  $x$ . As the integral is restricted to the area between the curves, the lower and upper bounds of the integral in  $x$  will depend on the particular value of  $y$ . The lower bound for integration over  $x$  is defined by the straight line so that  $x = \frac{y}{2}$  while the upper bound for integration over  $x$  is defined by the parabola so that  $x = \sqrt{y}$ . Integration over  $y$  follows integration over  $x$  with the lower and upper bounds of  $y = 0$  and  $y = 4$ , respectively.

With this understanding we can write a formula for the area between the curves in terms of the double integral<sup>19</sup>

$$\int_0^4 \int_{y/2}^{\sqrt{y}} dx dy = \int_0^4 \left[ \int_{y/2}^{\sqrt{y}} dx \right] dy$$

Evaluating the inner integral, we find

$$\int_0^4 \left[ \int_{y/2}^{\sqrt{y}} dx \right] dy = \int_0^4 \left[ x \right]_{y/2}^{\sqrt{y}} dy = \int_0^4 \left( \sqrt{y} - \frac{y}{2} \right) dy$$

We now have two definite integrals to complete, as

$$\int_0^4 \left( \sqrt{y} - \frac{y}{2} \right) dy = \left[ \frac{2}{3} y^{3/2} - \frac{1}{4} y^2 \right]_0^4 = \frac{2}{3} 4^{3/2} - \frac{1}{4} 4^2 = \frac{4}{3}$$

Conversely, this integral can also be evaluated by first integrating over  $y$  followed by integration over  $x$ :

$$\int_0^2 \int_{x^2}^{2x} dy dx = \int_0^2 \left[ \int_{x^2}^{2x} dy \right] dx = \int_0^2 (2x - x^2) dx = \frac{4}{3}$$

So we see that the order of integration does not matter. This will be true for most of the integrals of interest to us.

### 7.2.3 Double integrals of separable functions

The examples above demonstrate that integration over  $x$  and  $y$  can be coupled by integrating over areas that make the limits of integration over  $x$  dependent on  $y$  (and *vice versa*). However, integration over  $x$  and  $y$  can also be coupled when  $f(x, y)$  is a non-separable function of  $x$  and  $y$  and  $f(x, y) \neq g(x)h(y)$ .

Fortunately, most of the integrals of interest in the physical sciences are taken over *separable functions*. When  $f(x, y) = g(x)h(y)$  we can write

$$\begin{aligned} \int_c^d \int_a^b f(x, y) dx dy &= \int_c^d \int_a^b g(x)h(y) dx dy \\ &= \int_c^d h(y) dy \times \int_a^b g(x) dx \end{aligned}$$

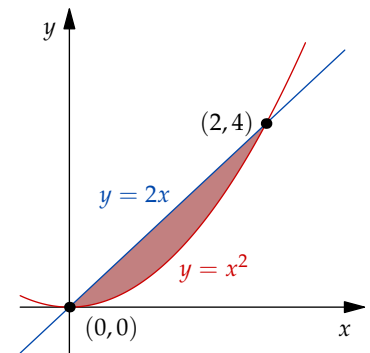


Figure 7.13: The curves defined by  $y = 2x$  (blue line) and  $y = x^2$  (red line) intersecting at the points  $(0,0)$  and  $(2,4)$  with the area between the curves shaded red.

<sup>19</sup>Note that we have taken the integrand to be unity.



This reduces the two-dimensional integral over the  $xy$ -plane to a product of two one-dimensional integrals. Separability will often depend on the right choice of coordinate systems. To better understand this critical idea, we will explore in detail a variety of examples involving the integration of separable functions of many variables.

### 7.2.4 Double integrals and the Tables of Integrals

A valuable application of integration in many dimensions involves determination of the area or volume of a geometric object. The area or volume can be determined by integration over the area or volume of the object where the integrand is unity.

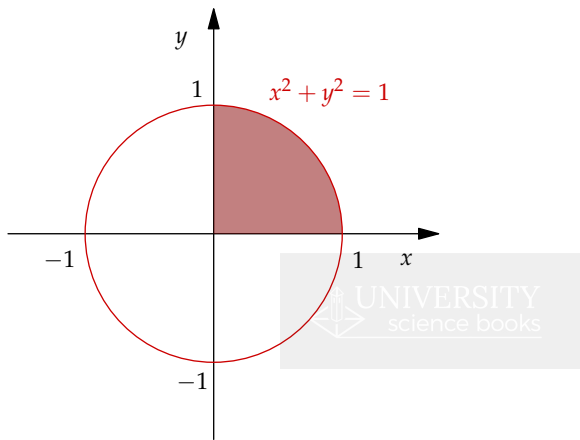


Figure 7.14: One quadrant of the unit circle with area equal to  $\frac{\pi}{4}$ .

Consider the evaluation of the area of a circle shown in Figure 7.14. We can divide and conquer this integral by first performing the integration over one quadrant. We then multiply that result by four. In that case, we wish to determine the shaded area of the quarter circle. The range of integration of  $x$  depends on the value of  $y$  as along the perimeter of the circle  $x = \sqrt{1 - y^2}$ . As such, the range of integration in  $x$  will have a lower bound of 0 and upper bound of  $x = \sqrt{1 - y^2}$ . The range of integration of  $y$  is from 0 to 1. With this understanding, we can write the integral over the quadrant as

$$\int_0^1 \int_0^{\sqrt{1-y^2}} dx dy = \int_0^1 \sqrt{1-y^2} dy$$

What do we do now? While we have reviewed methods for performing integrals of a single variable, nothing in our survey prepared us for this integral.

We will find that for many integrals of interest, the best way to solve them is to look up the result in a *table of integrals*.<sup>20</sup> Tables of definite and indefinite integrals sufficient to perform the problems in this text are included in Supplements S<sub>5</sub> and S<sub>6</sub>. These tables include the result

$$\int_0^a \sqrt{a^2 - x^2} dx = \left[ \frac{1}{2} \left[ x\sqrt{a^2 - x^2} + a^2 \sin^{-1} \left( \frac{x}{a} \right) \right] \right]_0^a$$

<sup>20</sup> The classic text is known as *Gradshteyn and Ryzhik* or simply GR which still serves as a valuable compendium of results for definite and indefinite integrals.

Izrail S. Gradshteyn and Iosif M. Ryzhik. *Table of Integrals, Series, and Products* [1943]. Academic Press, eighth edition, 2014. ISBN 0-12-384933-0

Using this result for our case of  $a = 1$ , we find

$$\int_0^1 \sqrt{1^2 - x^2} dx = \frac{1}{2} \sin^{-1}(1) = \frac{1}{4} \pi$$

This is the area over one quadrant of the unit circle. Four times this result is our answer to the original problem, to determine the area of the unit circle. The area of the unit circle is  $\pi$ .

### 7.2.5 Double integrals and the choice of coordinate system

The evaluation of the integral representing the area within the unit circle was somewhat complicated in cartesian coordinates. Cartesian coordinates have a natural square symmetry while the unit circle has round symmetry. Let's evaluate the integral again in plane polar coordinates, which better reflect the round symmetry of the unit circle.

Using the coordinate transformations explored in Chapter 1 and depicted in Figure 7.15, we can transform the integral over a quarter of the unit circle in two-dimensional cartesian coordinates to plane polar coordinates as

$$\begin{aligned} \int_0^1 \int_0^{\sqrt{1-y^2}} dx dy &= \int_0^{\pi/2} \int_0^1 r dr d\theta = \int_0^{\pi/2} d\theta \times \int_0^1 r dr \\ &= \frac{\pi}{2} \times \int_0^1 r dr = \frac{\pi}{2} \times \frac{1}{2} = \frac{\pi}{4} \end{aligned}$$

Multiplying this answer by 4 leads to the result that the area of the unit circle is  $\pi$ . However, in evaluating the integral in plane polar coordinates there is no need to break the integral into integrals over quarter circles as was required in cartesian coordinates. We can perform the integral at once over the whole unit circle as

$$\int_0^{2\pi} \int_0^1 r dr d\theta = \int_0^{2\pi} d\theta \times \int_0^1 r dr = 2\pi \times \int_0^1 r dr = 2\pi \times \frac{1}{2} = \pi$$

Much simpler! Note that in cartesian coordinates, the integrals over  $x$  and  $y$  were coupled through the limits of integration. In plane polar coordinates, the integrals over  $r$  and  $\theta$  are separable. The take home lesson is that the right choice of coordinate system, in which the variables reflect the natural symmetry of the function, can make the work of integration much easier.

### 7.2.6 Double integrals and the delta function

Suppose we want to determine the length of the circumference of a circle using an integral along the line forming the circle. We can accomplish this using the delta function. Let's start with the double integral over the  $xy$ -plane expressed in plane polar coordinates

$$\int_0^{2\pi} \int_0^{\infty} r dr d\theta$$

Now suppose we insert in the integrand  $\delta(r - a)$ . This makes the integrand zero unless  $r = a$ , which defines the perimeter of a circle. In that case, the integral over the  $xy$ -plane will be reduced to an integral over the perimeter of

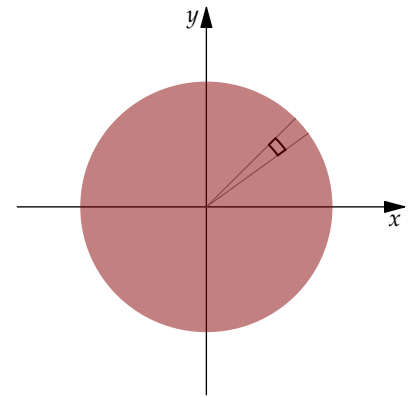


Figure 7.15: The plane polar coordinate system in two-dimensions showing the volume element  $dA = r dr d\theta$  (bold). The range of variables is defined by  $0 \leq r < \infty$  and  $0 \leq \theta < 2\pi$ .

the circle only. This gives us a formula for the circumference of the circle:

$$C = \int_0^{2\pi} \int_0^{\infty} \delta(r - a)r \, dr d\theta$$

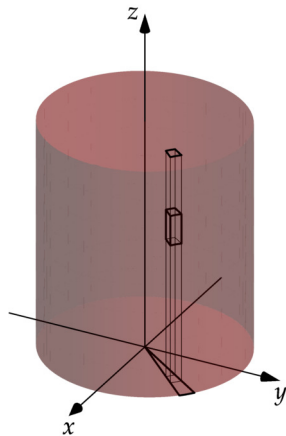
Performing the integral over  $r$  first,<sup>21</sup> followed by the integral over  $\theta$ , we find

$$\begin{aligned} \int_0^{2\pi} \int_0^{\infty} \delta(r - a)r \, dr d\theta &= \int_0^{2\pi} d\theta \times \int_0^{\infty} \delta(r - a)r \, dr \\ &= 2\pi \times \int_0^{\infty} \delta(r - a)r \, dr = 2\pi a \end{aligned}$$

which is the circumference of a circle of radius  $a$ . Inserting the delta function reduces the two-dimensional integral over the  $xy$ -plane to a one-dimensional integral over the perimeter of the circle.

### 7.2.7 Triple integrals

The evaluation of the volume of a solid is of fundamental importance in the physical sciences.<sup>22</sup> In order to extend our understanding of multiple integrals, let's consider the evaluation of the volume of a cylinder of radius  $a$  and height  $h$  (see Figure 7.16). Defining the volume of a cylinder in cartesian coordinates is complicated. The limits of integration in  $x$  and  $y$  are coupled just as we found in the integration over the unit circle. However, the integral over the volume of a cylinder can be naturally and simply expressed in using cylindrical coordinates.



The triple integral representing the volume of the cylinder can be written

$$\begin{aligned} V &= \int_0^h \int_0^{2\pi} \int_0^a r \, dr d\theta dz = \int_0^h dz \times \int_0^{2\pi} d\theta \times \int_0^a r \, dr \\ &= h \times 2\pi \times \frac{a^2}{2} = \pi a^2 h \end{aligned}$$

which is the intuitive result that the volume of the cylinder is equal to the circular area of the cylinder,  $\pi a^2$ , times the height  $h$ .

<sup>21</sup> Here we use the identity

$$\int_0^{\infty} \delta(r - a)r \, dr = a$$

where the Dirac delta function is zero everywhere other than the perimeter of the circle where  $r = a$ .

<sup>22</sup> Archimedes (circa 287-212 BCE) determined geometric volumes using the theory of *infinitesimals* before the concept of the integral was developed. The theory of infinitesimals was further applied to the calculation of areas and volumes by Johannes Kepler (1571-1630) in his 1615 treatise *New Solid Geometry of Wine Barrels*.

Figure 7.16: A cylinder of radius  $a$  and height  $h$ . Superimposed is the volume element  $dV = r dr d\theta dz$  (bold) with sides  $dr$ ,  $r d\theta$ , and  $dz$ . The range of variables is defined by  $0 \leq r < \infty$ ,  $0 \leq \theta < 2\pi$ , and  $-\infty < z < \infty$ .

Now suppose we want to determine the volume of a sphere. We want to select a coordinate system that shares the natural symmetry of a sphere. In cartesian coordinates, the limits of integration over  $x$ ,  $y$ , and  $z$  are coupled. However, the spherical polar coordinate system depicted in Figure 1.22 has the natural symmetry of a sphere. If we transform our function into spherical polar coordinates we find the integral is separable in  $r$ ,  $\theta$ , and  $\varphi$ :

$$\begin{aligned} V &= \int_0^{2\pi} \int_0^\pi \int_0^a r^2 \sin \theta \, dr d\theta d\varphi = \int_0^{2\pi} d\varphi \times \int_0^\pi \sin \theta d\theta \times \int_0^a r^2 \, dr \\ &= 2\pi \times 2 \times \frac{a^3}{3} = \frac{4}{3}\pi a^3 \end{aligned}$$

This is the well-known result for the volume of a sphere of radius  $a$ .<sup>23</sup>

These examples show how integration in three-dimensions can be used to derive important identities for volumes of shapes such as cylinders and spheres. Moreover, the examples show how the proper choice of coordinate system can convert a many dimensional integral into a series of independent one-dimensional integrations. For the integrals of greatest interest to us in the physical sciences, we will often find that multiple integrals can be simplified in this way.<sup>24</sup>

### 7.2.8 Triple integrals and the delta function

Suppose we want to determine the surface area of a sphere of radius  $a$ . We can accomplish this using the delta function. Let's start with the triple integral over all space in spherical polar coordinates

$$\int_0^{2\pi} \int_0^\pi \int_0^\infty f(r, \theta, \varphi) r^2 \sin \theta \, dr d\theta d\varphi$$

We insert into the integrand a function  $f(r, \theta, \varphi)$  that is zero everywhere in three-dimensional space other than on the surface of the sphere. We do that using the delta function

$$f(r, \theta, \varphi) = \delta(r - a)$$

which is zero everywhere other than on the spherical surface defined by  $r = a$ . As a result, we find the area of the surface of a sphere defined by the separable integral

$$\begin{aligned} \mathcal{A} &= \int_0^{2\pi} \int_0^\pi \int_0^\infty \delta(r - a) r^2 \sin \theta \, dr d\theta d\varphi \\ &= \int_0^{2\pi} d\varphi \times \int_0^\pi \sin \theta \, d\theta \times \int_0^\infty \delta(r - a) r^2 \, dr \end{aligned}$$

Performing the integral over  $r$  first, followed by the integrals over  $\theta$  and  $\varphi$ , we find

$$\mathcal{A} = a^2 \times \int_0^{2\pi} d\varphi \times \int_0^\pi \sin \theta \, d\theta = a^2 \times 2\pi \times 2 = 4\pi a^2$$

which is the area of the surface of a sphere of radius  $a$ . Inserting the delta function reduces the three-dimensional integral over all space to a two-dimensional integral over the surface of the sphere.

<sup>23</sup> We used the identity

$$\int_0^\pi \sin(x) dx = -[\cos x]_0^\pi = -(-1 - 1) = 2$$

to complete the integral over  $\theta$ .

<sup>24</sup> It is possible to extend the concept of the double and triple integrals to integrals over arbitrarily large numbers of variables. As large, in fact, as *Avogadro's number*, and larger still.

## A7 An alternative to integration by parts for exponential integrals

In exploring useful tricks for integrating functions of one variable, we performed integrals over an exponential function  $e^{ax}$  times a power of  $x$  of the form

$$\int x e^{ax} dx$$

To evaluate this integral, we used integration by parts where

$$\begin{aligned} u &= x & dv &= e^{ax} dx \\ du &= dx & v &= \frac{1}{a} e^{ax} \end{aligned} \tag{7.24}$$

This led to the result

$$\begin{aligned} \int x e^{ax} dx &= \frac{1}{a} x e^{ax} - \int \frac{1}{a} e^{ax} dx = \frac{1}{a} x e^{ax} - \frac{1}{a^2} e^{ax} \\ &= \frac{1}{a^2} (ax - 1) e^{ax} + C \end{aligned}$$

That was not too bad. However, consider the related integral

$$\int x^4 e^{ax} dx$$

To evaluate this integral using integration by parts, we need to apply the rule of integration by parts four times! Let's explore a way to improve our efficiency in performing integrals of this kind.

Consider the identity

$$x e^{ax} = \frac{d}{da} e^{ax}$$

where we have used the derivative with respect to the constant  $a$  to pull down a power of  $x$ . With this identity, we can rewrite the integral of interest as<sup>25</sup>

$$\int x e^{ax} dx = \frac{d}{da} \int e^{ax} dx$$

<sup>25</sup> We use the fact that

$$\frac{d}{da} \int f(ax) dx = \int \frac{df}{da} dx$$

Using our knowledge of the exponential integral, this integral can be evaluated as

$$\begin{aligned} \int x e^{ax} dx &= \frac{d}{da} \int e^{ax} dx = \frac{d}{da} \left( \frac{1}{a} e^{ax} \right) = -\frac{1}{a^2} e^{ax} + \frac{1}{a} x e^{ax} \\ &= \frac{1}{a^2} (ax - 1) e^{ax} + C \end{aligned} \tag{7.25}$$

just as we found using integration by parts.

The real power of this approach is evident in evaluating definite integrals over an exponential function  $e^{-ax}$  times a power of  $x$ . For example, we can readily evaluate the integral of  $x e^{-ax}$ :

$$\int_0^{\infty} x e^{-ax} dx = -\frac{d}{da} \int_0^{\infty} e^{-ax} dx = -\frac{d}{da} \frac{1}{a} = \frac{1}{a^2}$$

This result is consistent with the result derived with greater effort using integration by parts, where

$$\begin{aligned} u &= x & dv &= e^{-ax} dx \\ du &= dx & v &= -\frac{1}{a}e^{-ax} \end{aligned} \quad (7.26)$$

so that

$$\begin{aligned} \int_0^{\infty} x e^{-ax} dx &= -\frac{1}{a} x e^{-ax} \Big|_0^{\infty} - \int_0^{\infty} \left( -\frac{1}{a} e^{-ax} \right) dx \\ &= \frac{1}{a^2} e^{-ax} \Big|_0^{\infty} = \frac{1}{a^2} \end{aligned}$$

We see how our trick of differentiating with respect to  $a$  is more efficient than integration by parts for these particular definite integrals over the range  $0 \leq x \leq \infty$ . This is even more true for integrals such as

$$\int_0^{\infty} x^2 e^{-ax} dx = \frac{d^2}{da^2} \int_0^{\infty} e^{-ax} dx = \frac{d^2}{da^2} \frac{1}{a} = -\frac{d}{da} \frac{1}{a^2} = 2 \frac{1}{a^3}$$

This integral would require two rounds of integration by parts to be solved. Using our trick, we can solve the problem by simply differentiating the exponential twice with respect to  $a$ .



## B7 Evaluating the definite integral of a gaussian function

Consider the integral over the gaussian function

$$I = \int_{-\infty}^{\infty} e^{-ax^2} dx$$

There is no obvious way to evaluate this integral using our standard methods, such as algebraic substitution or integration by parts. Consider the algebraic substitution  $y = x^2$ . This leads to  $dy = 2x dx$ , introducing a factor of  $x$ . Similar problems arise in integration by parts, where the derivative of the gaussian function introduces a factor of  $x$ . To evaluate this integral, we will use an inspired trick imagined by the German mathematician *Carl Friedrich Gauss* for whom the gaussian function is now named.

Consider the product of two equivalent one-dimensional integrals

$$\int_{-\infty}^{\infty} e^{-ax^2} dx \times \int_{-\infty}^{\infty} e^{-ay^2} dy = I \times I = I^2$$

This product can be thought of as one two-dimensional integral over the  $xy$ -plane

$$I^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-a(x^2+y^2)} dx dy$$

This integral is most simply evaluated in plane polar coordinates, where

$$r^2 = x^2 + y^2 \quad \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy \rightarrow \int_0^{\infty} \int_0^{2\pi} r dr d\theta$$

With this transformation of variables, we arrive at the expression

$$\begin{aligned} I^2 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-a(x^2+y^2)} dx dy = \int_0^{\infty} \int_0^{2\pi} e^{-ar^2} r d\theta dr \\ &= 2\pi \int_0^{\infty} e^{-ar^2} r dr \end{aligned}$$

Defining  $u = r^2$ , so that  $du = 2r dr$ , results in

$$I^2 = 2\pi \int_0^{\infty} e^{-ar^2} r dr = \pi \int_0^{\infty} e^{-au} du = \pi \left[ -\frac{1}{a} e^{-au} \right]_0^{\infty} = \frac{\pi}{a}$$

leading to our final result

$$I = \int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

This result is recorded in the Table of Definite Integrals in Supplement S<sub>5</sub> #2. We commonly encounter integrals over gaussian functions in the physical sciences. As such, it is worthwhile to memorize this fundamental result.

## C<sub>7</sub> An alternative to integration by parts for gaussian integrals

We can extend our trick for efficiently integrating over integrands of the form  $x^n e^{-ax}$  to integrands of the form  $x^n e^{-ax^2}$  containing a gaussian function.

Consider the gaussian integral

$$\int_0^{\infty} e^{-ax^2} dx = \frac{1}{2} \int_{-\infty}^{\infty} e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}$$

Differentiating the gaussian function with respect to the parameter  $a$  pulls down a factor of  $-x^2$ . We find

$$\frac{d}{da} \int_0^{\infty} e^{-ax^2} dx = \int_0^{\infty} \frac{d}{da} e^{-ax^2} dx = - \int_0^{\infty} x^2 e^{-ax^2} dx$$

That means that

$$\begin{aligned} \int_0^{\infty} x^2 e^{-ax^2} dx &= -\frac{d}{da} \int_0^{\infty} e^{-ax^2} dx = -\frac{d}{da} \left( \frac{1}{2} \sqrt{\frac{\pi}{a}} \right) \\ &= \frac{1}{4a^{3/2}} \sqrt{\pi} \end{aligned}$$

For the odd powers of  $x$ , we can start from the integral identity<sup>26</sup>

$$\int_0^{\infty} x e^{-ax^2} dx = \frac{1}{2a}$$

and use our trick to show

$$\int_0^{\infty} x^3 e^{-ax^2} dx = -\frac{d}{da} \int_0^{\infty} x e^{-ax^2} dx = -\frac{d}{da} \left( \frac{1}{2a} \right) = \frac{1}{2a^2}$$

While integrals of this form can be evaluated using integration by parts, the

<sup>26</sup> We can evaluate the integral

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

with the algebraic substitution  $y = x^2$  so that  $dy = 2x dx$  and

$$I = \frac{1}{2} \int_0^{\infty} e^{-ay} dy = \frac{1}{2a}$$

effort required is significant. Using our trick, we can most efficiently evaluate integrals over gaussian functions that commonly occur in the physical sciences.

## D7 Properties of delta functions

Delta functions can be used to select specific terms in a series or points in a function. Here we explore the properties of two delta functions that are commonly used in the physical sciences, the Kronecker delta function and the Dirac delta function.

### Kronecker delta function

The *Kronecker delta function*,  $\delta_{nm}$ , is a function of two discrete indices  $n$  and  $m$ . It is defined to be zero except when  $n = m$ :

$$\delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases}$$

This function is used in sums to select those terms for which two indices are equal (see Figure 7.17).<sup>27</sup> For example, consider the sum

$$\sum_{n=-\infty}^{\infty} a_n \delta_{nm} = a_m$$

where  $\delta_{nm}$  is used to select only the elements  $a_n$  for which  $n = m$ . This is known as the *sifting property*.

The Kronecker delta function is normalized as

$$\sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \delta_{nm} = 1$$

These examples demonstrate how the Kronecker delta function can be used to sift through and select specific terms in a finite or infinite series.

### Dirac delta function

The *Dirac delta function*,  $\delta(x - x_0)$ , is zero everywhere except at the point  $x = x_0$ , where it is infinite:

$$\delta(x - x_0) = \begin{cases} \infty & x = x_0 \\ 0 & x \neq x_0 \end{cases}$$

This function is used in integrals to select a particular value of the variable  $x$  (see Figure 7.18). For example, consider the integral

$$\int_{-\infty}^{\infty} f(x) \delta(x - x_0) = f(x_0)$$

where  $\delta(x - x_0)$  is used to select the single value of the function  $f(x)$  for which  $x = x_0$ . This is the *sifting property* observed for the Kronecker delta function.

<sup>27</sup> The German mathematician *Leopold Kronecker* (1902-1984) made important contribution to number theory and logic.

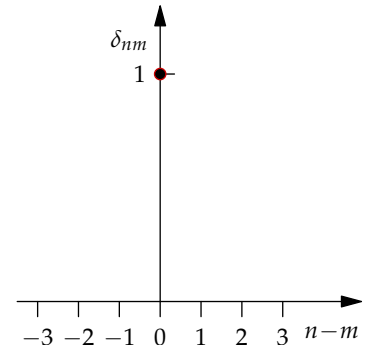


Figure 7.17: The Kronecker delta function  $\delta_{nm}$  as a function of the difference between the indices  $n$  and  $m$ .



The Dirac delta function is normalized as

$$\int_{-\infty}^{\infty} \delta(x - x_0) = 1$$

and can be defined in terms of the first derivative of the *Heaviside step function*,  $\theta(x - x_0)$ , which is 0 for  $x < x_0$  and unity for  $x \geq x_0$  (see Figure 7.5).

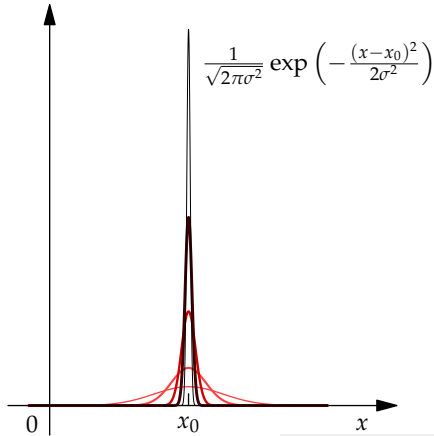


Figure 7.18: The normalized gaussian function centered at  $x_0$  with decreasing values of  $\sigma$  ranging from large (pale red line) to small (black line). In the limit that  $\sigma \rightarrow 0$ , the function approaches the Dirac delta function  $\delta(x - x_0)$ .

There is a rich variety of ways to represent the Dirac delta function. In problem solving in the physical sciences, one representation of the delta function might lead to an easier solution than another representation. One popular representation of the delta function is defined in terms of a normalized gaussian function with its standard deviation  $\sigma$  approaching zero, represented by the limit

$$\delta(x - x_0) = \lim_{\sigma \rightarrow 0} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-x_0)^2}{2\sigma^2}} \quad (7.27)$$

This function is continuous and differentiable with a maximum at  $x = x_0$ . As  $\sigma \rightarrow 0$ , the function's height increases toward infinity, according to  $1/\sigma$ , while its width decreases to zero, according to  $\sigma$ , preserving the normalization

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-x_0)^2}{2\sigma^2}} dx = 1$$

for all values of  $\sigma$ . This gaussian function is shown in Figure 7.18 for values of the parameter  $\sigma$  ranging from 0.5 to 0.025.

These observations provide a guide to designing other representations of the Dirac delta function. We need a function that is normalized with a single parameter that controls the width and height of the function such that in some limit the function becomes infinitely tall and infinitesimally wide.

Let's consider the *lorentzian function*

$$\delta(x - x_0) = \frac{1}{\pi} \lim_{\sigma \rightarrow 0} \frac{\sigma}{(x - x_0)^2 + \sigma^2} \quad (7.28)$$

Like the gaussian function, it is continuous and differentiable, with a height

proportional to  $1/\sigma$  and width proportional to  $\sigma$  so that the area normalized for all values of  $\sigma$  (see Supplement S<sub>5</sub>#13). This lorentzian function is shown in Figure 7.19 for values of the parameter  $\sigma$  ranging from 1 to 0.05.

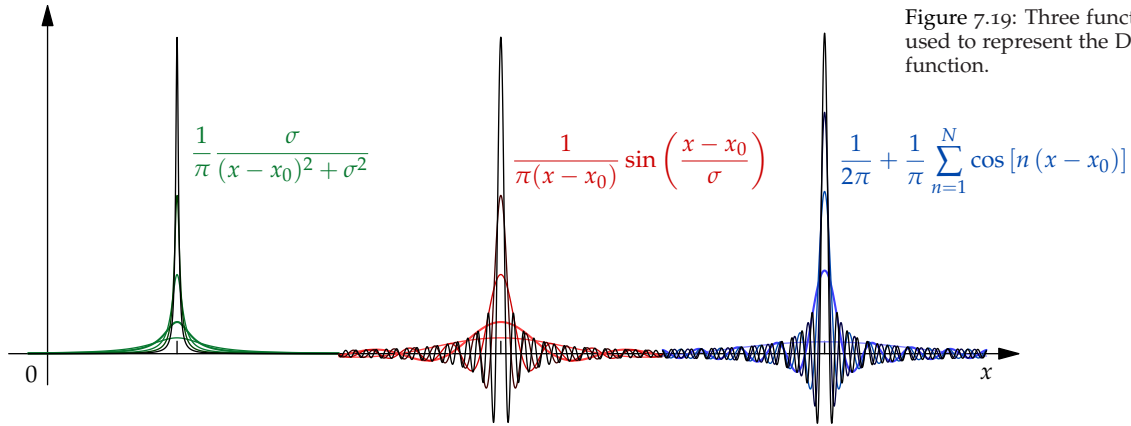


Figure 7.19: Three functional forms used to represent the Dirac delta function.

Less obvious functional representations of the Dirac delta function make use of sine or cosine terms. Consider the sinusoidal function

$$\delta(x - x_0) = \frac{1}{\pi} \lim_{\sigma \rightarrow 0} \frac{1}{(x - x_0)} \sin\left(\frac{x - x_0}{\sigma}\right) \quad (7.29)$$

This function is normalized, since

$$\int_{-\infty}^{\infty} \frac{1}{(x - x_0)} \sin\left(\frac{x - x_0}{\sigma}\right) dx = \pi$$

independent of the parameter  $\sigma$  (see the Table of Definite Integrals in Supplement S<sub>5</sub>). This is surely one of the more remarkable definitions of the mathematical constant  $\pi$ . The height of the function at  $x = x_0$  increases according to  $1/\sigma$  as  $\sigma$  decreases, and the width of the function decreases in proportion to  $\sigma$ . This function is shown in Figure 7.19 for values of the parameter  $\sigma$  ranging from 1 to 0.05.

The Dirac delta function can also be expressed as an infinite cosine series:

$$\delta(x - x_0) = \frac{1}{2\pi} + \lim_{N \rightarrow \infty} \frac{1}{\pi} \sum_{n=1}^N \cos[n(x - x_0)] \quad (7.30)$$

Note that this formulation is independent of a parameter  $\sigma$  controlling the height and width of the function. The increased height and decreased width are realized through the constructive and destructive interference between terms of the cosine series. This function is shown in Figure 7.19 for values of the parameter  $N$  ranging from 1 to 40.

The Dirac delta function is useful in modeling a point charge, point mass, or electron. These examples show a few of the many ways the Dirac delta function can be represented in terms of continuous and differentiable functions of one variable. Many other examples exist and some can be found in Chapter 13, which explores Fourier transforms and harmonic analysis.

## E7 End-of-chapter problems

I consider that I understand an equation when I can predict the properties of its solutions, without actually solving it.

Paul Dirac

### Warm-ups

7.1 Evaluate the following indefinite integrals. Consider italicized letters other than the integration variable to be constants. Include the integration constant  $C$  in your result.

$$\begin{array}{lll}
 \text{(a)} \int mv \, dv & \text{(b)} \int \frac{1}{x^3} \, dx & \text{(c)} \int \sin 3x \, dx \\
 \text{(d)} \int (3x + 5)^2 4x \, dx & \text{(e)} \int e^{-\varepsilon/k_B T} \, d\varepsilon & \text{(f)} \int \cos(2\pi vt) \, dt \\
 \text{(g)} \int \frac{RT}{p} \, dp & \text{(h)} \int \frac{1}{2} \kappa x^2 \, dx & \text{(i)} \int \frac{q^2}{4\pi\epsilon_0 r^2} \, dr
 \end{array}$$

7.2 Evaluate the following integrals, using various methods of integration and the tables integrals found in Supplements S<sub>5</sub> and S<sub>6</sub> as needed. Consider italicized letters other than the integration variable to be constants. Include the integration constant  $C$  in your result.

$$\begin{array}{lll}
 \text{(a)} \int \cos(5x) \cos(3x) \, dx & \text{(b)} \int x^4 e^{-ax} \, dx & \text{(c)} \int \sin^2\left(\frac{n\pi x}{L}\right) \, dx \\
 \text{(d)} \int \frac{dx}{(a-x)^n} & \text{(e)} \int y e^{-y^2/2\sigma^2} \, dy & \text{(f)} \int e^{-\gamma x} \sin x \, dx \\
 \text{(g)} \int \frac{dx}{(4-x)(3-x)} & \text{(h)} \int \cos^3 \varphi \sin \varphi \, d\varphi & \text{(i)} \int x^3 \cos 2x \, dx
 \end{array}$$

7.3 Evaluate the following definite integrals, using the tables of integrals found in Supplements S<sub>5</sub> and S<sub>6</sub> as needed. Consider italicized letters other than the integration variable to be constants.

$$\begin{array}{lll}
 \text{(a)} \int_{-\infty}^{\infty} x^3 e^{-ax^2} \, dx & \text{(b)} \int_{p_1}^{p_2} \frac{RT}{p} \, dp & \text{(c)} \int_{V_1}^{V_2} \left( \frac{nRT}{V-nb} - \frac{n^2 a}{V^2} \right) \, dV \\
 \text{(d)} \int_0^L x^2 \sin^2\left(\frac{n\pi x}{L}\right) \, dx & \text{(e)} \int_{T_1}^{T_2} \frac{\Delta H}{RT^2} \, dT & \text{(f)} \int_{T_1}^{T_2} \left( a + bT + cT^2 + \frac{d}{T} \right) \, dT \\
 \text{(g)} \int_0^{\infty} e^{-2r/a_0} r \, dr & \text{(h)} \int_0^{\infty} e^{-mv^2/2kT} v^3 \, dv & \text{(i)} \int_0^{\infty} (2J+1) e^{-a(J^2+J)} \, dJ
 \end{array}$$

7.4 Evaluate the following multiple integrals, using the tables of integrals found in Supplements S<sub>5</sub> and S<sub>6</sub> as needed. For indefinite integrals be sure to include an integration constant.

$$\text{(a)} \iint yx^2 \, dx \, dy \qquad \text{(b)} \iint (x^2 + y^2) \, dx \, dy$$

(c)  $\iint y \ln x \, dy \, dx$

(d)  $\iiint x^2 \ln y e^{2x} \, dx \, dy \, dz$

(e)  $\int_0^{\pi/2} \int_0^2 r \cos \theta \, dr \, d\theta$

(f)  $\int_0^{2\pi} \int_0^\pi \int_0^V v^2 \sin \theta \, dv \, d\theta \, d\varphi$

(g)  $\int_0^\infty \int_0^\infty (x^2 + y^2) e^{-\frac{1}{2}(x^2+y^2)} \, dx \, dy$

(h)  $\int_{-\infty}^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty e^{-\frac{1}{2k_B T}(mv_x^2 + mv_y^2 + mv_z^2)} \, dv_x \, dv_y \, dv_z$

*Homework exercises*

7.5 Evaluate the following integral, which commonly appears in quantum mechanics and statistical thermodynamics

$$I = \int_0^\pi (3 \cos^2 \theta - 1)^2 \sin \theta \, d\theta$$

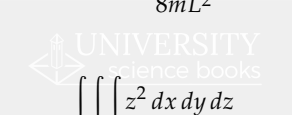
7.6 The allowed energies of a quantum mechanical particle in a one-dimensional box of length  $L$  can be written

$$E_n = -\frac{\hbar^2}{2m} \frac{2}{L} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \left[ \frac{d^2}{dx^2} \sin\left(\frac{n\pi x}{L}\right) \right] dx$$

where  $n = 1, 2, 3, \dots$  and  $\hbar = h/2\pi$  is the constant  $h$  bar. Complete the integral to show that

$$E_n = \frac{n^2 \hbar^2}{8mL^2}$$

7.7 Consider the integral



$$\iiint z^2 \, dx \, dy \, dz$$

taken over the volume of a sphere of radius  $a$ . Using spherical polar coordinates where  $z = r \cos \theta$  the integral takes the form

$$\int_0^a \int_0^\pi \int_0^{2\pi} (r \cos \theta)^2 r^2 \sin \theta \, d\varphi \, d\theta \, dr$$

Evaluate this integral.

7.8 Consider the integral over all space

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} e^{-2r} \cos^2 \theta r^2 \sin \theta \, d\varphi \, d\theta \, dr$$

Evaluate this integral.

7.9 Consider the integral

$$\iiint xyz \, dx \, dy \, dz$$

taken over the volume defined by  $0 \leq z < a$  and  $x^2 + y^2 \leq b^2$  where  $x \geq 0$  and  $y \geq 0$ . This integral can be expressed in cylindrical coordinates as

$$\int_0^a \int_0^{\frac{\pi}{2}} \int_0^b (r^2 \cos \theta \sin \theta) z r \, dr \, d\theta \, dz$$

Evaluate this integral.

7.10 Consider a gas of atoms interacting with a pairwise *square well potential* energy function dependent on the

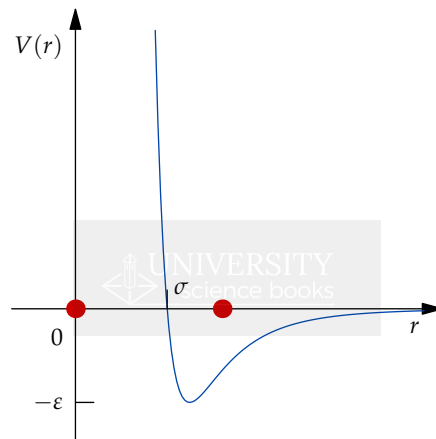
distance  $r$  between a pair of atoms

$$V(r) = \begin{cases} \infty & 0 < r \leq \sigma \\ -\varepsilon & \sigma < r \leq \lambda\sigma \\ 0 & r > \lambda\sigma \end{cases}$$

where  $\lambda > 1$  controls the width of the well of depth  $\varepsilon$ . The potential function is shown below (red line) and compared with the smooth Lennard-Jones potential energy function (blue line) examined in Chapter 5 (see Figure 5.12). The *compressibility factor* of the gas can be written as a Taylor's series expansion in powers of the number of density  $n/V$  as

$$Z = \frac{PV}{nRT} = 1 + B(T)\frac{n}{V} + C(T)\left(\frac{n}{V}\right)^2 + \text{higher order terms}$$

This is known as the *virial expansion* where the coefficients  $B(T)$  and  $C(T)$  are the second and third virial coefficients, respectively.



The second virial coefficient is defined as

$$B(T) = -\frac{1}{2} \int_0^\infty \int_0^\pi \int_0^{2\pi} \left( e^{-\beta V(r)} - 1 \right) r^2 \sin \theta \, d\varphi \, d\theta \, dr$$

where  $\beta = 1/k_B T$ .

(a) Plot the potential energy  $V(r)$  as a function of  $r$  over the range  $0 < r < 2\lambda\sigma$  taking  $\lambda = 2$ .

(b) Show that  $B(T)$  can be written

$$B(T) = -2\pi \int_0^\infty \left( e^{-\beta V(r)} - 1 \right) r^2 \, dr$$

(c) Evaluate the integral in (b) to show that

$$B(T) = \frac{2\pi\sigma^3}{3} \left[ 1 - (\lambda^3 - 1)(e^{\beta\varepsilon} - 1) \right]$$

(d) Take the limit of your result as  $\lambda \rightarrow 1$  and provide a physical interpretation of that limit.

7.11 Prove that

$$I_n = \int_0^{\infty} r^n e^{-\beta r} dr = \frac{n!}{\beta^{n+1}}$$

This result is recorded in the Table of Definite Integrals in Supplement S<sub>5</sub> #1.

7.12 Starting from the result that

$$I_0 = \int_0^{\infty} e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}$$

show that

$$I_{2n} = \int_0^{\infty} x^{2n} e^{-ax^2} dx = \frac{(2n-1)!!}{2^{n+1} a^n} \sqrt{\frac{\pi}{a}}$$

where the *double factorial* is defined

$$(2n-1)!! = (2n-1)(2n-3) \dots 3 \cdot 1$$

This result is recorded in the Table of Definite Integrals in Supplement S<sub>5</sub> #4.

7.13 Starting from the result that

$$I_1 = \int_0^{\infty} x e^{-ax^2} dx = \frac{1}{2a}$$

show that

$$I_{2n+1} = \int_0^{\infty} x^{2n+1} e^{-ax^2} dx = \frac{n!}{2a^{n+1}}$$

This result is recorded in the Table of Definite Integrals in Supplement S<sub>5</sub> #7.

7.14\* The Dirac delta function is defined as

$$\delta(x - x_0) = \begin{cases} 0 & x \neq x_0 \\ \infty & x = x_0 \end{cases}$$

such that

$$\int_{-\infty}^{\infty} \delta(x - x_0) dx = 1$$

and

$$\int_{-\infty}^{\infty} \delta(x - x_0) f(x) dx = f(x_0)$$

Evaluate the following integrals involving the Dirac delta function.

(a)  $I = \int_0^{2\pi} \delta(\theta - \pi) \cos \theta d\theta$

(b)  $I = \int_0^{\infty} \delta(t - 1) e^{-t} dt$

(c)  $I = \int_0^{\infty} \int_0^{2\pi} \delta(r - a) r d\theta dr$

(d)  $I = \int_{-2L}^{2L} \int_{-2L}^{2L} \delta(x - L) dx dy$

(e)  $I = \int_{-2L}^{2L} \int_{-2L}^{2L} \int_{-2L}^{2L} \delta(y + L) dx dy dz$

(f)  $I = \int_{-\infty}^{\infty} \delta(x - 1) (x^2 - 1)^2 dx$

7.15\* In Chapter 1, we considered the transformation of a volume element from one coordinate system to another. For example, using geometric arguments we found the volume element in two-dimensional cartesian coordinates,  $dA = dx dy$  in Figure 1.14, is transformed to  $dA = r dr d\theta$  in two-dimensional plane polar coordinates (see Figure 1.18). This exercise explores a systematic approach for transforming a volume element between coordinate systems that draws on our knowledge of partial derivatives and the determinant.

Suppose we start from the volume element  $dA = dx dy$  in two-dimensional cartesian coordinates. That volume

element can be transformed to plane polar coordinates using the formula

$$dxdy = |\mathbf{J}| drd\theta$$

where  $|\mathbf{J}|$  is the determinant of the *jacobian matrix* defined

$$\mathbf{J} = \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{pmatrix} = \frac{\partial(x, y)}{\partial(r, \theta)}$$

The mapping between  $(x, y)$  and  $(r, \theta)$  is defined by

$$x = r \cos \theta \quad y = r \sin \theta$$

so that the determinant of the jacobian matrix is

$$|\mathbf{J}| = \begin{vmatrix} \cos \theta & -r \sin \theta \\ \sin \theta & r \cos \theta \end{vmatrix} = r \cos^2 \theta + r \sin^2 \theta = r$$

resulting in

$$dxdy = |\mathbf{J}| drd\theta = r drd\theta$$

So you see how it works.

(a) Write the jacobian matrix for the transformation from three-dimensional cartesian coordinates  $(x, y, z)$  to spherical polar coordinates  $(r, \theta, \varphi)$  defined by

$$dxdydz = |\mathbf{J}| drd\theta d\varphi = \left| \frac{\partial(x, y, z)}{\partial(r, \theta, \varphi)} \right| drd\theta d\varphi$$

Evaluate the determinant of the jacobian matrix to show that the volume element  $dV = r^2 \sin \theta drd\theta d\varphi$ .

(b) Write the jacobian matrix for the transformation from three-dimensional cartesian coordinates  $(x, y, z)$  to cylindrical coordinates  $(r, \theta, z)$  defined by

$$dxdydz = |\mathbf{J}| drd\theta dz = \left| \frac{\partial(x, y, z)}{\partial(r, \theta, z)} \right| drd\theta dz$$

Evaluate the determinant of the jacobian matrix to show that the volume element  $dV = r drd\theta dz$ .