# Appendix A. Some Mathematical Tools of Quantum Mechanics

## A. Calculus with One Variable

Quantum Mechanics takes extensive advantage of calculus, and you should familiarize yourself with techniques of calculus. The two basic functions of calculus are the derivative and the integral. The derivative of a function of one variable $f(x)$ can be written as $df(x)/dx$ or $f'(x)$. Finding derivatives of most functions is not difficult. The following table gives derivatives of the most common simple functions

$$\frac{d}{dx}c = 0 \qquad \frac{d}{dx}\sin x = \cos x \qquad \frac{d}{dx}\sin^{-1}(x) = \frac{1}{\sqrt{1-x^2}}$$

$$\frac{d}{dx}x^n = nx^{n-1} \qquad \frac{d}{dx}\cos x = -\sin x \qquad \frac{d}{dx}\cos^{-1}(x) = -\frac{1}{\sqrt{1-x^2}}$$

$$\frac{d}{dx}e^x = e^x \qquad \frac{d}{dx}\tan x = \sec^2 x \qquad \frac{d}{dx}\tan^{-1}(x) = \frac{1}{1+x^2}$$

$$\frac{d}{dx}\ln x = \frac{1}{x}$$

Notice that many other functions can be rewritten in terms of these functions; for example, $\sqrt{x} = x^{1/2}$ and $1/x = x^{-1}$. In addition, there are rules for taking the derivatives of sums, differences, products, quotients, and composition of functions:

$$\frac{d}{dx}\left[f(x) \pm g(x)\right] = f'(x) \pm g'(x)$$

$$\frac{d}{dx}\left[f(x)g(x)\right] = f'(x)g(x) + f(x)g'(x)$$

$$\frac{d}{dx}\left[\frac{f(x)}{g(x)}\right] = \frac{f'(x)g(x) - f(x)g'(x)}{g^2(x)}$$

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

As a special case, note that when a function has a constant added to it, the constant has no effect; when a function has a constant multiplied by it, the constant simply multiplies the derivative as well.

The other thing you do in the calculus of one variable is to integrate. There are two types of integrals, definite and indefinite. A definite integral has limits of integration and is defined as the area under a specific curve between two limits. It looks like this:

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

 

The other type of integral is an indefinite integral. It uses the same symbol, except that no limits are specified, and it is defined as the anti-derivative; that is, the function whose derivative is $f(x)$. In other words, if we let $F(x)$ be the indefinite integral of $f(x)$, then

$$F(x) = \int f(x)\,dx \Leftrightarrow F'(x) = f(x)$$

As we already mentioned, if you add a constant to a function *F*, its derivative is unchanged, so that the indefinite integral is ambiguous up to an additive constant. Hence, in general, the indefinite integrals should always end with $+C$, an unknown constant. The fundamental theorem of calculus tells us that these two types of integrals are related. Specifically, if the indefinite integral of $f(x)$ is $F(x)$, then

$$\int_a^b f(x)\,dx = \int_a^b F'(x)\,dx = F(x)\Big|_a^b = F(b) - F(a) \qquad \text{(A.1)}$$

Because of the subtraction, the constant of integration cancels out, and therefore is unnecessary and irrelevant when calculating an indefinite integral. Note that if you ever have to exchange the two limits of an integral, the resulting integral changes sign, as is clear from (A.1). Also note that in any definite integral, the variable being integrated (*x* in this case) disappears after the substitution of the limits, and hence can be replaced by any other unused variable with impunity.

Unlike derivatives, there are no simple rules for doing integrals. Generally you use a few steps to try to convert your integral into smaller, more manageable pieces, and then either look up the integral in an integral table, or use some tool like Maple to do the integral. Two of the simple rules that allow you to convert complicated integrals into simpler ones are

$$\int cf(x)\,dx = c\int f(x)\,dx$$
$$\int \left[f(x) \pm g(x)\right]dx = \int f(x)\,dx \pm \int g(x)\,dx$$

In addition, it is possible to change variables. Suppose we have an integral and we wish to change variables $x = g(y)$. Then we can substitute this integral in to find

$$\int f(x)\,dx = \int f\big(g(y)\big)\,d\left[g(x)\right] = \int f\big(g(y)\big)\,g'(y)\,dy$$

Note that if you are dealing with an indefinite integral, you will have to substitute back in to convert to the original variable *x* using $y = g^{-1}(x)$. If you are doing a definite integral, this may not be necessary, but you will have to redo the limits of integration appropriately.

Once the equation has been massaged into a relatively well-controlled form, you will often be left with some integrals that you need to complete. I recommend looking them up in an integral table or using a program like Maple. For example, suppose you have the surprisingly difficult integral

$$\int_{-\infty}^{\infty} \exp\left(-Ax^2\right)dx$$

 

This integral is defined only if $A$ is positive; otherwise, the integral is undefined. To determine the integral, you must tell Maple that this constant is positive. To find this integral, open Maple, and then enter the commands[1]

```
> assume(A>0);integrate(exp(-A*x^2),x=-infinity..infinity);
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and it will come back with the answer

$$\int_{-\infty}^{\infty} \exp\left(-Ax^2\right) dx = \sqrt{\pi/A}\,.$$

A very useful formula from the calculus of one variable is the Taylor expansion, which says that a function in the neighborhood of any point $a$ can be expanded in terms of the value of the function and its derivatives at the point $a$. The Taylor expansion is

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

where $n!$ is defined as $1 \cdot 2 \cdot 3 \cdots n$. This formula will strictly speaking be true only if the function $f$ is sufficiently smooth between $a$ and $x$, and if the sum converges. If the sum does *not* converge, a finite sum often will still serve as an excellent approximation for the function, though it will not be perfect.

The Taylor expansion comes up in lots of situations, but it is most commonly used for a power of $1+x$, for $e^x$, and for $\cos x$ and $\sin x$. For these functions, the Taylor expansion gives

$$(1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \frac{n(n-1)(n-2)}{3!}x^3 + \cdots \tag{A.2a}$$

$$e^x = \exp(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \tag{A.2b}$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots \tag{A.2c}$$

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots \tag{A.2d}$$

The notation $\exp(x)$ is an alternate notation for $e^x$, useful because we will often make the argument of this function quite complicated, and it is easier to read, for example, $\exp\left(-\tfrac{1}{2}Ax^2\right)$ then it is to read $e^{-\frac{1}{2}Ax^2}$. (A.2a) is convergent for any complex number $|x|<1$; the other three converge for all complex $x$. Another nice feature about the equations (A.2) is that if we replace $x$ with any square matrix, the formulas still make sense, so we can now take exponentials of matrices, for example. Euler's theorem, which we will use extensively, can be derived from (A.2b), (A.2c), and (A.2d):

$$e^{ix} = \exp(ix) = \cos x + i \sin x\,. \tag{A.3}$$

[1]To make the input look like this (which I find much more readable than the default format), you must be in worksheet mode, and then click on Tools, Options, Display, and change the Input Display to Maple Input. Click on Apply Globally and your results will look like mine.

B. Calculus with Several Variables

In math we often work in one dimension; in physics, at least when we are doing realistic calculations, there are at least three. A *scalar function* in three dimensions would be a single ordinary function like $f(\mathbf{r}) = f(x, y, z)$. A *vector function* in three dimensions would actually be a triplet of functions $\mathbf{A}(\mathbf{r})$, with

$$\mathbf{A}(\mathbf{r}) = \hat{\mathbf{x}}A_x(\mathbf{r}) + \hat{\mathbf{y}}A_y(\mathbf{r}) + \hat{\mathbf{z}}A_z(\mathbf{r}), \tag{A.4}$$

where $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ are unit vectors in the directions of increasing *x*, *y*, and *z* respectively. We can then take the derivatives of scalar functions or the components of vector functions using partial derivative, which we write as $\partial/\partial x$, $\partial/\partial y$, and $\partial/\partial z$.[1] It is helpful to define a sort of vector derivative, which we denote as

$$\nabla \equiv \hat{\mathbf{x}}\frac{\partial}{\partial x} + \hat{\mathbf{y}}\frac{\partial}{\partial y} + \hat{\mathbf{z}}\frac{\partial}{\partial z}$$

This vector derivative, in three dimensions, can be used to produce a vector function from a scalar function using the gradient, defined by

$$\nabla f \equiv \hat{\mathbf{x}}\frac{\partial f}{\partial x} + \hat{\mathbf{y}}\frac{\partial f}{\partial y} + \hat{\mathbf{z}}\frac{\partial f}{\partial z} \tag{A.5}$$

From a vector function $\mathbf{A}(\mathbf{r})$, we can product a scalar function by using the divergence, defined as

$$\nabla \cdot \mathbf{A} \equiv \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}. \tag{A.6}$$

We also define the curl, a vector quantity, as

$$\nabla \times \mathbf{A} \equiv \hat{\mathbf{x}}\left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right) + \hat{\mathbf{y}}\left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right) + \hat{\mathbf{z}}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) \tag{A.7}$$

Finally, it is useful to define the Laplacian, a second derivative of a scalar function, given by

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \tag{A.8}$$

The gradient, divergence, and Laplacian, generalize in an obvious way to higher dimensions; the curl, in contrast, does not so simply generalize.

Just as you can take derivatives for functions of multiple variables, you can also do integrals. We will focus almost exclusively on volume integrals, which are a type of

[1] Note that in this notation, expressions like $f'(\mathbf{r})$ make no sense. We must either write out the partial derivative explicitly, or develop a new, more sophisticated shorthand.

definite integral where we add up the value of some function $f(\mathbf{r})$ over a volume *V*. A volume integral would be written something like

$$\iiint_V f(\mathbf{r})\,dV = \iiint_V f(\mathbf{r})\,d^3\mathbf{r}$$

Such an integral is really *three* one dimensional integrals, one over each of the three Cartesian coordinates *x*, *y*, and *z*. Writing out more explicitly, you can think of the integral as of the form

$$\iiint_V f(\mathbf{r})\,d^3\mathbf{r} = \int dx \int dy \int dz\; f(x,y,z) \tag{A.9}$$

In other words, we have three nested integrals, one inside the other (they can generally be performed in any order). As set up here, one would first perform the inner *z* integral, then the intermediate *y* integral, and finally the outermost *x* integral. The limits can be quite tricky; for example, the innermost integral (*z*) may have limits that depend on the outer two variable (*x* and *y*), while the intermediate integral may have limits that depend on the outermost variable (*x*), but not the inner variable (*z*), and the outermost integral (*x*) may not depend on the other two variables. Furthermore, when performing the integral, the variables *x* and *y* should be treated as constants inside the inner-most integral, while *z* is a variable; when you perform the intermediate integral, *y* is a variable, *x* is a constant, and *z* should have disappeared, and in the outermost integral, only the variable *x* should appear.

For example, suppose that I were given a region *V* defined by the four conditions

$$V = \left\{(x,y,z) : x > 0, y > 0, z > 0, x + y + z < 1\right\}$$

Now, suppose I was asked to find the volume of this region, which is

$$\iiint_V 1 d^3\mathbf{r} = \int dx \int dy \int dz$$

What limits should I use? For the innermost integral, the simultaneous conditions $z > 0$ and $x + y + z < 1$ set the interval of integration as $(0, 1 - x - y)$. For the intermediate integration, we don't know what *z* is (other than positive), but clearly $y > 0$ and $x + y < 1$, and for the outermost integration, we know only that $0 < x < 1$. So the correct limits are

$$\begin{aligned}\iiint_V 1 d^3\mathbf{r} &= \int_0^1 dx \int_0^{1-x} dy \int_0^{1-x-y} dz = \int_0^1 dx \int_0^{1-x} (1 - x - y)\,dy \\ &= \int_0^1 dx \left(y - xy - \tfrac{1}{2}y^2\right)\Big|_{y=0}^{y=1-x} = \int_0^1 dx\left[(1-x)^2 - \tfrac{1}{2}(1-x)^2\right] \\ &= \tfrac{1}{2}\int_0^1 (1-x)^2\,dx = -\tfrac{1}{6}(1-x)^3\Big|_{x=0}^{1} = \tfrac{1}{6}\end{aligned}$$

As a notational matter, it is worth noting that when given a multidimensional integral, it is common to use only a single integral symbol, rather than the triple integral. If the integral is over all space, it is common to leave the limit symbol *V* out of it entirely.

 

Is there any multi-dimensional analog of the fundamental theorem of calculus, (A.5), that allows you to find the integral of a derivative? There are several, in fact, depending on what type of integral you are dealing with. The one we will need most often is Gauss's Law, which relates an integral over a volume *V* to a surface integral over the boundary of *V* when you are integrating a divergence of a vector function.

$$\iiint_V \nabla \cdot \mathbf{A}(\mathbf{r})\, dV = \oiint_S \hat{\mathbf{n}} \cdot \mathbf{A}(\mathbf{r})\, dS , \tag{A.10}$$

where *S* is the boundary of the volume *V* and $\hat{\mathbf{n}}$ is a unit normal sticking out of the integration region. The funky integral symbol on the right side of (A.10) merely indicates that the integral is being taken over a closed surface. The reason (A.10) still has integrals left over is because we started with a triple integral, and the derivative 'cancels' only one of the integrals, leaving you still with the two-dimensional surface integral. Equation (A.10) generalizes easily to other dimensions as well. In particular, in one dimension, the left side has only a single integral, and the right side is not an integral, but merely surface terms coming from the two limits of integration. In other words, the one-dimensional version of (A.10) is (A.1).

Stokes' Theorem will also prove useful. It relates the integral of the curl of a vector field over a surface to an integral around the boundary of that same surface:

$$\iint_S \hat{\mathbf{n}} \cdot \left[\nabla \times \mathbf{A}(\mathbf{r})\right] dS = \oint_C \mathbf{A}(\mathbf{r}) \cdot d\mathbf{l} \tag{A.11}$$

Once again, the number of integrals is reduced by one.

Finally, there is the divergence theorem, which assists you in performing a path integral of the divergence of a function from one point to another along a path:

$$\int_A^B \left[\nabla f(\mathbf{r})\right] \cdot d\mathbf{l} = f(B) - f(A) \tag{A.12}$$

## C. Coordinates in Two and Three Dimensions

In dimensions higher than one, it is common to use alternate coordinates besides the conventional Cartesian coordinates. When you change coordinates from a set of coordinates $(x_1, x_2, \ldots, x_N)$ to a new set of coordinates $(y_1, y_2, \ldots, y_N)$, any integration over the *N*-dimensional volume must be transformed as well. The rule is

$$\int f(\mathbf{x})\, d^N\mathbf{x} = \int f(\mathbf{x}(\mathbf{y})) \left|\det\left(\partial x_i / \partial y_i\right)\right| d^N\mathbf{y} \tag{A.13}$$

Furthermore, all of the derivative operators must be rewritten in the new basis as well.

Let's start with two dimensions. In addition to standard Cartesian coordinates $(x, y)$, the most common set of coordinates are polar coordinates $(\rho, \phi)$. The relations between these two coordinate systems are

$$\begin{Bmatrix} x = \rho\cos\phi \\ y = \rho\sin\phi \end{Bmatrix} \qquad \text{and} \qquad \begin{Bmatrix} \rho = \sqrt{x^2 + y^2} \\ \phi = \tan^{-1}(y/x) \end{Bmatrix} \tag{A.14}$$

For any pair $(x, y)$ there are multiple values of $(\rho, \phi)$ that satisfy these equations. To make the relationship (A.14) unambiguous, we therefore restrict the coordinates $(\rho, \phi)$ by

$$\begin{aligned} &0 \le \rho \\ &0 \le \phi < 2\pi \end{aligned} \tag{A.15}$$

The inverse tangent must be considered carefully, since there will be two values of $\phi$ in the range $0 \le \phi < 2\pi$ that satisfy $\phi = \tan^{-1}(y/x)$. The ambiguity can be removed with the help of $y = \rho\sin\phi$: we choose $0 < \phi < \pi$ if $y$ is positive and $\pi < \phi < 2\pi$ if $y$ is negative. If $y$ vanishes, then we pick $\phi = 0$ if $x$ is positive and $\phi = \pi$ if $x$ is negative. If $x$ and $y$ both vanish, then $\phi$ is ambiguous; it is a bad spot in the coordinate system.

Scalar functions in one coordinate system are unchanged in the new coordinate system, but a vector quantity will now take the form

$$\mathbf{A} = \hat{\boldsymbol{\rho}} A_\rho + \hat{\boldsymbol{\varphi}} A_\phi$$

These components can be related to the ordinary Cartesian components by

$$\begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} A_\rho \\ A_\phi \end{pmatrix}, \qquad \begin{pmatrix} A_\rho \\ A_\phi \end{pmatrix} = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix} \tag{A.16}$$

We present, without proof, formulas for the gradient, divergence, Laplacian, and integral in these new coordinates:

$$\nabla f = \frac{\partial f}{\partial \rho}\hat{\boldsymbol{\rho}} + \frac{1}{\rho}\frac{\partial f}{\partial \phi}\hat{\boldsymbol{\varphi}} \tag{A.17a}$$

$$\nabla \cdot \mathbf{A} = \frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho A_\rho\right) + \frac{1}{\rho}\frac{\partial A_\phi}{\partial \phi} \tag{A.17b}$$

$$\nabla^2 f = \frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho\frac{\partial f}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 f}{\partial \phi^2} \tag{A.17c}$$

$$\iint f(\mathbf{r})\, d^2\mathbf{r} = \int \rho\, d\rho \int d\phi\, f(\rho, \phi) \tag{A.17d}$$

If one integrates over all space, the limits of integration in (A.17d) are implied by (A.15).

In three dimensions, there are two coordinate systems that are commonly used in addition to Cartesian. The first are cylindrical, where $(x, y, z)$ are replaced with $(\rho, \phi, z)$, defined by the relations

$$\begin{Bmatrix} x = \rho\cos\phi \\ y = \rho\sin\phi \\ z = z \end{Bmatrix} \quad \text{and} \quad \begin{Bmatrix} \rho = \sqrt{x^2+y^2} \\ \phi = \tan^{-1}(y/x) \\ z = z \end{Bmatrix} \tag{A.18}$$

where the last expression in each triplet means simply that the coordinate $z$ is unchanged. These coordinates are obviously very similar to polar coordinates in two dimensions. The restrictions (A.15) apply in this case as well, and the inverse tangent must be interpreted carefully in a manner similar to the comments after (A.15). Vector functions in the two coordinates are related in a manner almost identical to (A.9):

$$\begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} A_\rho \\ A_\phi \\ A_z \end{pmatrix}, \qquad \begin{pmatrix} A_\rho \\ A_\phi \\ A_z \end{pmatrix} = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix}$$

The various differential and integral relations look nearly identical to (A.16), except we include the curl:

$$\nabla f = \frac{\partial f}{\partial \rho}\hat{\boldsymbol{\rho}} + \frac{1}{\rho}\frac{\partial f}{\partial \phi}\hat{\boldsymbol{\phi}} + \frac{\partial f}{\partial z}\hat{\mathbf{z}} \tag{A.19a}$$

$$\nabla\cdot\mathbf{A} = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho A_\rho\right) + \frac{1}{\rho}\frac{\partial A_\phi}{\partial\phi} + \frac{\partial A_z}{\partial z} \tag{A.19b}$$

$$\nabla\times\mathbf{A} = \left(\frac{1}{\rho}\frac{\partial A_z}{\partial\phi} - \frac{\partial A_\phi}{\partial z}\right)\hat{\boldsymbol{\rho}} + \left(\frac{\partial A_\rho}{\partial z} - \frac{\partial A_z}{\partial\rho}\right)\hat{\boldsymbol{\phi}} + \frac{1}{\rho}\left(\frac{\partial}{\partial\rho}\left(\rho A_\phi\right) - \frac{\partial A_\rho}{\partial\phi}\right)\hat{\mathbf{z}} \tag{A.19c}$$

$$\nabla^2 f = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial f}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 f}{\partial\phi^2} + \frac{\partial^2 f}{\partial z^2} \tag{A.19d}$$

$$\iiint f(\mathbf{r})\,d^3\mathbf{r} = \int \rho\,d\rho \int d\phi \int dz\; f(\rho,\phi,z) \tag{A.19e}$$

Spherical coordinates $(r,\theta,\phi)$ are related to Cartesian coordinates by the relations

$$\begin{Bmatrix} x = r\sin\theta\cos\phi \\ y = r\sin\theta\sin\phi \\ z = r\cos\theta \end{Bmatrix} \quad \text{and} \quad \begin{Bmatrix} r = \sqrt{x^2+y^2+z^2} \\ \theta = \tan^{-1}\left(\sqrt{x^2+y^2}/z\right) \\ \phi = \tan^{-1}(y/x) \end{Bmatrix}, \tag{A.20}$$

with coordinate restrictions

$$\begin{aligned} &0 \le r \\ &0 \le \theta \le \pi \\ &0 \le \phi < 2\pi \end{aligned}$$

The ambiguity in the variable $\phi$ is resolved in a manner identical to that in polar coordinates in two dimensions or cylindrical in three. There is no corresponding ambiguity for $\theta$. They are related to cylindrical coordinates by

$$\begin{Bmatrix} \rho = r\sin\theta \\ \phi = \phi \\ z = r\cos\theta \end{Bmatrix} \quad \text{and} \quad \begin{Bmatrix} r = \sqrt{\rho^2 + z^2} \\ \theta = \tan^{-1}(\rho/z) \\ \phi = \phi \end{Bmatrix} \tag{A.21}$$

Vector functions in spherical coordinates are related to Cartesian by

$$\begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi & \cos\theta\cos\phi & -\sin\phi \\ \sin\theta\sin\phi & \cos\theta\sin\phi & \cos\phi \\ \cos\theta & -\sin\theta & 0 \end{pmatrix} \begin{pmatrix} A_r \\ A_\theta \\ A_\phi \end{pmatrix},$$

$$\begin{pmatrix} A_r \\ A_\theta \\ A_\phi \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix}$$

and they are related to cylindrical coordinates by

$$\begin{pmatrix} A_\rho \\ A_\phi \\ A_z \end{pmatrix} = \begin{pmatrix} \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \\ \cos\theta & -\sin\theta & 0 \end{pmatrix} \begin{pmatrix} A_r \\ A_\theta \\ A_\phi \end{pmatrix}, \qquad \begin{pmatrix} A_r \\ A_\theta \\ A_\phi \end{pmatrix} = \begin{pmatrix} \sin\theta & 0 & \cos\theta \\ \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} A_\rho \\ A_\phi \\ A_z \end{pmatrix}.$$

The various differential and integral identities in this coordinate system look like

$$\nabla f = \frac{\partial f}{\partial r}\hat{\mathbf{r}} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\boldsymbol{\theta}} + \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\hat{\boldsymbol{\varphi}} \tag{A.22a}$$

$$\nabla \cdot \mathbf{A} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 A_r\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(A_\theta \sin\theta\right) + \frac{1}{r\sin\theta}\frac{\partial A_\phi}{\partial \phi} \tag{A.22b}$$

$$\nabla \times \mathbf{A} = \frac{1}{r\sin\theta}\left[\frac{\partial}{\partial\theta}\left(A_\phi \sin\theta\right) - \frac{\partial A_\theta}{\partial\phi}\right]\hat{\mathbf{r}} + \frac{1}{r}\left(\frac{1}{\sin\theta}\frac{\partial A_r}{\partial\phi} - \frac{\partial}{\partial r}\left(rA_\phi\right)\right)\hat{\boldsymbol{\theta}} + \frac{1}{r}\left(\frac{\partial}{\partial r}\left(rA_\theta\right) - \frac{\partial A_r}{\partial\theta}\right)\hat{\boldsymbol{\varphi}} \tag{A.22c}$$

$$\nabla^2 f = \frac{1}{r}\frac{\partial^2}{\partial r^2}(rf) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2} \tag{A.22d}$$

$$\iiint f(\mathbf{r})\,d^3\mathbf{r} = \int r^2 dr \int \sin\theta d\theta \int d\phi\, f(r,\theta,\phi) \tag{A.22e}$$

The Laplacian can also be rewritten as

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2} \tag{A.23}$$

D. Special Functions

Certain types of functions come up commonly enough in physics that you should become familiar with them. One has already been encountered, the factorial, defined by

$$0! = 1$$
$$n! = 1\cdot 2\cdot 3\cdots n$$

A closely related function is the Gamma function, usually defined as

$$\Gamma(n) = \int_0^\infty x^{n-1} e^{-x} dx \tag{A.24}$$

It is not hard to show by integration by parts that this satisfies the recursion relationship

$$\Gamma(n+1) = n\Gamma(n) \tag{A.25}$$

This relationship together with the easily derived fact that $\Gamma(1) = 1$ allows you to prove that if *n* is a positive integer, then

$$\Gamma(n+1) = n!$$

The reason the Gamma function is more generally useful is that (A.13) can be defined also for non-integers, indeed for any positive number or even any complex number with a positive real part. Indeed, with the help of (A.25), you can extend the definition to *all* complex numbers (except for zero and negative integers, for which $\Gamma(n)$ diverges). In particular, half-integers come up a lot, and it is helpful to know that

$$\Gamma\left(\tfrac{1}{2}\right) = \sqrt{\pi} \tag{A.26}$$

Together with (A.25), you can use this to get $\Gamma(n)$ for any half-integer *n*. Equation (A.26) can be proven with the help of a Gaussian integral, to which we turn next.

A simple Gaussian is a function of the form

$$e^{-Ax^2}$$

For *A* real and positive, this function peaks at the origin, and quickly dies out as *x* goes to positive or negative infinity. If *A* is complex but has a positive real part, it still has a maximum magnitude at the origin, but it will not only diminish but also rotate in the complex plane as you move away from zero. We very often will encounter Gaussian integrals of the form

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

A clever trick allows us to evaluate this integral. First square it, writing the right side as the integral times itself, and then change the variable of integration of one of the two resulting integral from *x* to *y*:

$$I^2 = \left[\int_{-\infty}^{\infty} e^{-Ax^2} dx\right]^2 = \left[\int_{-\infty}^{\infty} e^{-Ax^2} dx\right]\left[\int_{-\infty}^{\infty} e^{-Ay^2} dy\right] = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-Ax^2-Ay^2} dx\, dy$$

Now change this two-dimensional area integral into polar coordinates with the help of (A.17d)

$$I^2 = \int_0^{2\pi} \int_0^{\infty} e^{-A\rho^2} \rho d\rho \, d\phi$$

The $\phi$ integral is trivial, and the $\rho$ integral is remarkably easy

$$I^2 = 2\pi \frac{1}{2A} \int_0^{\infty} e^{-A\rho^2} d\left(A\rho^2\right) = -\frac{\pi}{A} e^{-A\rho^2}\Big|_0^{\infty} = \frac{\pi}{A}$$

Taking the square root, we have $I = \sqrt{\pi/A}$, so in conclusion

$$\int_{-\infty}^{\infty} e^{-Ax^2} dx = \sqrt{\frac{\pi}{A}} \text{ for } \operatorname{Re}(A) \geq 0 \tag{A.27}$$

Since $A$ might be complex, we should clarify that the square root is chosen such that the real part is positive. The formula also works for $A$ pure imaginary, provided $A$ is not zero. If you let $A$ = 1 and substitute $x = \sqrt{y}$, in (A.27), it is not hard to derive (A.26).

Starting from (A.27), it isn't hard to derive a more general integral, which I call a shifted Gaussian, given by

$$\int_{-\infty}^{\infty} e^{-Ax^2 + Bx} dx = \sqrt{\frac{\pi}{A}} \exp\left(\frac{B^2}{4A}\right) \text{ for } \operatorname{Re}(A) \geq 0 \tag{A.28}$$

If there are extra powers of $x$ in front, it is possible to see that these can be found by taking derivatives of (A.28) with respect to $B$, since this brings down factors of $x$. Hence we have

$$\int_{-\infty}^{\infty} x^n e^{-Ax^2 + Bx} dx = \sqrt{\frac{\pi}{A}} \frac{\partial^n}{\partial B^n} \left[\exp\left(\frac{B^2}{4A}\right)\right] \text{ for } \operatorname{Re}(A) \geq 0 \tag{A.29}$$

This formula takes a particular simple form if $B$ = 0. Though it can be derived directly from (A.29), it is easier to change variables and use the definition of the Gamma function to show that

$$\int_{-\infty}^{\infty} x^n e^{-Ax^2} dx = \Gamma\left(\tfrac{n+1}{2}\right) A^{-\frac{n+1}{2}} \quad \text{for } n \text{ even} \tag{A.30}$$

For $n$ odd, the integral vanishes because the positive and negative parts cancel out.

Some additional functions that come up occasionally are hyperbolic functions. Three of them are defined as

$$\cosh(x) = \tfrac{1}{2}\left(e^x + e^{-x}\right)$$
$$\sinh(x) = \tfrac{1}{2}\left(e^x - e^{-x}\right)$$
$$\tanh(x) = \frac{\sinh(x)}{\cosh(x)}$$

Like $e^{\pm x}$, both cosh and sinh satisfy the differential equation $f''(x) = f(x)$. However, they are even and odd functions respectively. Indeed, using Euler's Theorem (A.3), it is easy to see that these are closely related to the trigonometric functions through the complex numbers; specifically

$$\cosh(ix) = \cos(x)$$
$$\sinh(ix) = i\sin(x)$$
$$\tanh(ix) = i\tan(x)$$

## E. The Dirac Delta function

One other function requires special attention, though strictly speaking, it isn't a function at all. The Dirac delta function is written $\delta(x)$, and is defined to be the function such that for any function $f(x)$, we have

$$\int_{-\infty}^{\infty} f(x)\delta(x)\,dx = f(0) \tag{A.31}$$

You should think of the Dirac delta function as a function that vanishes everywhere except the origin, but it is infinitely large at the origin, and has a total area of 1. As such, it is not, in the mathematical sense, a function at all (sometimes it is called a 'distribution'), but we can think of it as the limit of a peak with very narrow width and very large height. For example, consider the limit

$$\delta(x) \equiv \lim_{A\to\infty} \sqrt{\frac{A}{\pi}} e^{-Ax^2} \tag{A.32}$$

For large but finite *A*, this represents a function whose height is very large, but which quickly diminishes outside of a small region surrounding the origin. If, for example, the function $f(x)$ is continuous near the origin, its value will change little in the region where $\delta(x)$ is large, and we can treat it as a constant $f(x) \approx f(0)$ in this region. We can therefore demonstrate that (A.31) implies (A.32) because

$$\begin{aligned} \int_{-\infty}^{\infty} f(x)\delta(x)\,dx &= \lim_{A\to\infty}\int_{-\infty}^{\infty} f(x)\sqrt{A/\pi}\, e^{-Ax^2}dx = f(0)\lim_{A\to\infty}\sqrt{A/\pi}\int_{-\infty}^{\infty} e^{-Ax^2}dx \\ &= f(0)\sqrt{A/\pi}\sqrt{\pi/A} = f(0) \end{aligned} \tag{A.33}$$

This is not to imply that (A.32) is the *only* way to define the Dirac delta function. Furthermore, the arguments given assume that the function $f(x)$ is continuous at the origin; if this is not the case, then the integral (A.31) will not work, and indeed, the integral is poorly defined.

Several variants of (A.31) will prove useful. First of all, because the only place that contributes to the integral is the origin, (A.31) will remain true if we change the upper and lower limits of integration, provided 0 is still within the range of integration (if it isn't, the integral is just 0). We can shift the argument of the delta function, which simply shifts the point where we evaluate the function *f*:

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

We can even imagine having functions inside the Dirac delta function. Suppose we are given an integral of the form

$$\int_{-\infty}^{\infty} f(x)\delta\big(g(x)\big)\,dx \tag{A.34}$$

For the moment, let us assume that $g(x)$ is a monotonic function, which either increases from $-\infty$ to $+\infty$ as *x* increases, or decreases from $+\infty$ to $-\infty$. The key to performing this integration is to define a new variable $y = g(x)$, and rewrite the integral in terms of *y*. We imagine finding the inverse function $x = g^{-1}(y)$. The result will be

$$\int_{-\infty}^{\infty} f(x)\delta\big(g(x)\big)dx = \int_{-\infty}^{\infty} f\big(g^{-1}(y)\big)\delta(y)\,dx = \int_{g^{-1}(-\infty)}^{g^{-1}(\infty)} f\big(g^{-1}(y)\big)\delta(y)\frac{dx}{dy}dy \tag{A.35}$$

Now, suppose for the moment that *g* is an increasing function, and therefore the limits are exactly as before, $-\infty$ to $+\infty$. Then this integral is straightforward, and we have

$$\int_{-\infty}^{\infty} f(x)\delta\big(g(x)\big)dx = f\big(g^{-1}(y)\big)\frac{dx}{dy}\bigg|_{y=0} = \frac{f\big(g^{-1}(0)\big)}{\left[dy/dx\right]_{y=0}} = \frac{f\big(g^{-1}(0)\big)}{g'\big(g^{-1}(0)\big)} \quad \text{if } g \text{ is increasing} \tag{A.36}$$

where $g'$ is the derivative of *g*. Note that in this case, $g'$ is positive everywhere. On the other hand, if *g* is a decreasing function, the limits on the final integral in (A.35) will be switched, which produces a minus sign. If you work through the same steps as we did in (A.36), you find

$$\int_{-\infty}^{\infty} f(x)\delta\big(g(x)\big)dx = -\frac{f\big(g^{-1}(0)\big)}{g'\big(g^{-1}(0)\big)} \qquad \text{if } g \text{ is decreasing} \tag{A.37}$$

Note that in this case, $g'$ is negative everywhere. We can therefore combine equations (A.36) and (A.37) into a single case, which we write as

$$\int_{-\infty}^{\infty} f(x)\delta\big(g(x)\big)dx = \frac{f(x_1)}{\left|g'(x_1)\right|} \qquad \text{for } g \text{ increasing or decreasing} \tag{A.38}$$

where $x_1 = g^{-1}(0)$; *i.e.*, the unique point where $g(x_1) = 0$.

What do we do if the function *g* does not go from $-\infty$ to $+\infty$, or vice versa, but instead has only a finite range, or perhaps even turns around and is sometimes increasing and sometimes decreasing? The answer can be understood by thinking more carefully about the integral (A.34). Recall that the Dirac delta function vanishes except when its argument is zero. Therefore, if $g(x)$ doesn't vanish anywhere, the integral (A.23) vanishes. If $g(x)$ vanishes at one point, but doesn't go all the way to $-\infty$ or $+\infty$, it doesn't matter; just as in (A.31), the upper and lower limits don't matter, so long as the range includes 0. Equation (A.38) is still valid. If $g(x)$ vanishes more than once, then each time it vanishes there will be a contribution to the integral (A.38), and that contribution will be of the form (A.38), so as a consequence the result will be a sum.

$$\int_{-\infty}^{\infty} f(x)\,\delta\big(g(x)\big)\,dx = \sum_i \frac{f(x_i)}{\left|g'(x_i)\right|} \tag{A.39}$$

$x_i$ are all the solutions of $g(x_i) = 0$

Indeed, if the upper and lower limits of (A.39) are changed, the right hand side will remain unchanged, except that the sum will be restricted to those roots of $g$ which lie within the range of integration. Equation (A.39) can be rewritten in non-integral form as

$$\delta\big(g(x)\big) = \sum_i \frac{\delta(x - x_i)}{\left|g'(x_i)\right|}, \quad x_i \text{ are all the solutions of } g(x_i) = 0\,. \tag{A.40}$$

As an example, suppose $g(x) = x^2 - a^2$, then $g'(x) = 2x$, and the two roots of $g(x) = 0$ are $x = \pm a$, and we find

$$\int_{-\infty}^{\infty} f(x)\,\delta\left(x^2 - a^2\right)dx = \frac{1}{2a}\left[f(a) + f(-a)\right]$$

The Dirac delta function can be generalized to more than one dimension by simply multiplying one-dimensional Dirac delta functions. In three dimensions,

$$\delta^3(\mathbf{r}) \equiv \delta(x)\,\delta(y)\,\delta(z)$$

It easily follows that

$$\iiint f(\mathbf{r})\,\delta^3(\mathbf{r} - \mathbf{a})\,d^3\mathbf{r} = f(\mathbf{a})$$

Analogs of (A.39) and (A.40) can be derived for when the Dirac delta function has a vector argument, $\delta^3\big(\mathbf{g}(\mathbf{r})\big)$. We give the results without proof.

$$\iiint f(\mathbf{r})\,\delta\big(\mathbf{g}(\mathbf{r})\big)\,d^3\mathbf{r} = \sum_i \frac{f(\mathbf{r}_i)}{\left|\det\left[\partial\mathbf{g}(\mathbf{r}_i)/\partial\mathbf{r}\right]\right|} \tag{A.41a}$$

$$\delta^3\big(\mathbf{g}(\mathbf{r})\big) = \sum_i \frac{\delta^3(\mathbf{r} - \mathbf{r}_i)}{\left|\det\left[\partial\mathbf{g}(\mathbf{r}_i)/\partial\mathbf{r}\right]\right|} \tag{A.41b}$$

where $\mathbf{r}_i$ are all the roots of $\mathbf{g}(\mathbf{r}_i) = \mathbf{0}$ and the determinants are taken with respect to the three by three matrix which results when you take the derivative of the three components of **g** with respect to the three coordinate components **r**.

## F. Fourier Transforms

We start with the following "identity":

$$\int_{-\infty}^{\infty} e^{ikx} dx = 2\pi\delta(k) \tag{A.42}$$

This identity cannot really be proven, simply because it isn't quite true, but it can be justified by considering the following integral, which can be evaluated with the help of (A.28):

$$\lim_{\varepsilon\to 0^+} \int_{-\infty}^{\infty} e^{ikx-\varepsilon x^2} dx = \sqrt{\frac{\pi}{\varepsilon}} \exp\left(\frac{(ik)^2}{4\varepsilon}\right) = \lim_{\varepsilon\to 0^+} \sqrt{\frac{\pi}{\varepsilon}} \exp\left(-\frac{k^2}{4\varepsilon}\right)$$

Let $\varepsilon = 1/4A$ and use (A.32) to simplify, so that we have

$$\int_{-\infty}^{\infty} e^{ikx} dx = \lim_{A\to\infty} \sqrt{4\pi A} \exp\left(-Ak^2\right) = \sqrt{4\pi^2}\,\delta(k) = 2\pi\delta(k)$$

Strictly speaking, the interchange of the limit with the integration is not valid, but this formula is so widely used in physics that we will treat it as true.

Let $f(x)$ be any reasonably smooth function. We will normally also demand that $f$ vanish not too slowly, say, faster than $1/x$ at large $x$. Then define the Fourier transform $\tilde{f}(k)$ as

$$\tilde{f}(k) \equiv \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} f(x) e^{-ikx}$$

Consider now the Fourier transform of the Fourier transform, which we will evaluate with the help of (A.42)

$$\begin{aligned}\tilde{\tilde{f}}(x) &= \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \tilde{f}(k) e^{ikx} = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty} f(y) e^{iky} dy\right] e^{ikx} dk \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty} e^{ik(x+y)} dk\right] f(y)\,dy = \int_{-\infty}^{\infty} \delta(x+y) f(y)\,dy = f(-x)\end{aligned}$$

Up to sign, the Fourier transform of a Fourier transform is the function back again. We therefore summarize this information as two relations, here presented together.

$$\begin{aligned}\tilde{f}(k) &= \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} f(x) e^{-ikx} \\ f(x) &= \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \tilde{f}(k) e^{ikx}\end{aligned} \tag{A.43}$$

One other relation that is not hard to prove is that the magnitude squared integral of a function and its Fourier transform are the same. The proof is given below.

$$\int_{-\infty}^{\infty}\left|\tilde{f}(k)\right|^2 dk = \int_{-\infty}^{\infty}\tilde{f}(k)^*\,\tilde{f}(k)\,dk = \int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}\,f(x)e^{-ikx}dx\right]\left[\int_{-\infty}^{\infty}\frac{dy}{\sqrt{2\pi}}\,f(y)e^{-iky}dy\right]^* dk$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x)\,dx\int_{-\infty}^{\infty} f^*(y)\,dy\int_{-\infty}^{\infty} dk e^{-ikx}e^{iky}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x)\,dx\int_{-\infty}^{\infty} f^*(y)\,dy\,(2\pi)\,\delta(y-x) = \int_{-\infty}^{\infty} f(x)\,f^*(x)\,dx,$$

$$\int_{-\infty}^{\infty}\left|\tilde{f}(k)\right|^2 dk = \int_{-\infty}^{\infty}\left|f(x)\right|^2 dx \tag{A.44}$$

All of these formulas can be generalized to three (or more) dimensions easily, so we give the resulting equations without proof.

$$\iiint e^{i\mathbf{k}\cdot\mathbf{r}}d^3\mathbf{r} = (2\pi)^3\,\delta^3(\mathbf{k}) \tag{A.45a}$$

$$\tilde{f}(\mathbf{k}) = \iiint\frac{d^3\mathbf{r}}{(2\pi)^{3/2}}f(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{A.45b}$$

$$f(\mathbf{r}) = \iiint\frac{d^3\mathbf{k}}{(2\pi)^{3/2}}\tilde{f}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}} \tag{A.45c}$$

$$\iiint\left|\tilde{f}(\mathbf{k})\right|^2 d^3\mathbf{k} = \iiint\left|f(\mathbf{r})\right|^2 d^3\mathbf{r} \tag{A.45d}$$