Mathematical background 1 Differentiation and integration

Two of the most important mathematical techniques in the physical sciences are differentiation and integration. They occur throughout the subject, and it is essential to be aware of the procedures involved.

MB1.1 Differentiation: definitions

Differentiation is concerned with the slopes of functions, such as the rate of change of a variable with time. The formal definition of the **derivative**, $\mathrm{d}f/\mathrm{d}x$, of a function $f(x)$ is

$$\frac{\mathrm{d}f}{\mathrm{d}x}=\lim_{\delta x\to 0}\frac{f(x+\delta x)-f(x)}{\delta x}$$ *Definition* First derivative (MB1.1)

As shown in Fig. MB1.1, the derivative can be interpreted as the slope of the tangent to the graph of $f(x)$. A positive first derivative indicates that the function slopes upwards (as x increases), and a negative first derivative indicates the opposite. It is sometimes convenient to denote the first derivative as $f'(x)$. The **second derivative**, $\mathrm{d}^2f/\mathrm{d}x^2$, of a function is the derivative of the first derivative (here denoted f'):

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}=\lim_{\delta x\to 0}\frac{f'(x+\delta x)-f'(x)}{\delta x}$$ *Definition* Second derivative (MB1.2)

It is sometimes convenient to denote the second derivative f''. As shown in Fig. MB1.1, the second derivative of a function can be interpreted as an indication of the sharpness of the curvature of the function. A positive second derivative indicates that the function is ∪ shaped, and a negative second derivative indicates that it is ∩ shaped.

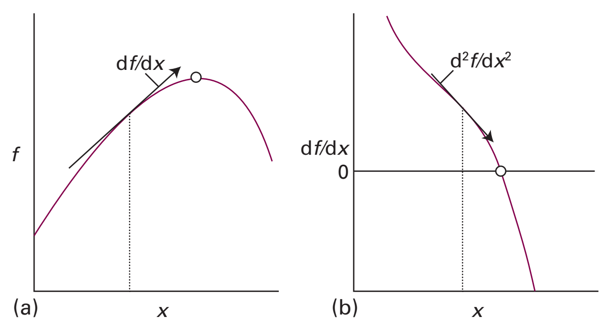

Figure MB1.1 (a) The first derivative of a function is equal to the slope of the tangent to the graph of the function at that point. The small circle indicates the extremum (in this case, maximum) of the function, where the slope is zero. (b) The second derivative of the same function is the slope of the tangent to a graph of the first derivative of the function. It can be interpreted as an indication of the curvature of the function at that point.

The derivatives of some common functions are as follows:

$$\frac{\mathrm{d}}{\mathrm{d}x}x^n=nx^{n-1}\qquad\text{(MB1.3a)}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{ax}=a\mathrm{e}^{ax}\qquad\text{(MB1.3b)}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\sin ax=a\cos ax\qquad\frac{\mathrm{d}}{\mathrm{d}x}\cos ax=-a\sin ax\qquad\text{(MB1.3c)}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\ln ax=\frac{1}{x}\qquad\text{(MB1.3d)}$$

When a function depends on more than one variable, we need the concept of a **partial derivative**, $\partial f/\partial x$. Note the change from d to ∂: partial derivatives are dealt with at length in *Mathematical background* 2; all we need know at this stage is that they signify that all variables other than the stated variable are regarded as constant when evaluating the derivative.

Brief illustration MB1.1 Partial derivatives

Suppose we are told that f is a function of two variables, and specifically $f=4x^2y^3$. Then, to evaluate the partial derivative of f with respect to x, we regard y as a constant (just like the 4), and obtain

$$\frac{\partial f}{\partial x}=\frac{\partial}{\partial x}(4x^2y^3)=4y^3\frac{\partial}{\partial x}x^2=8xy^3$$

Similarly, to evaluate the partial derivative of f with respect to y, we regard x as a constant (again, like the 4), and obtain

$$\frac{\partial f}{\partial y}=\frac{\partial}{\partial y}(4x^2y^3)=4x^2\frac{\partial}{\partial y}y^3=12x^2y^2$$

MB1.2 Differentiation: manipulations

It follows from the definition of the derivative that a variety of combinations of functions can be differentiated by using the following rules:

$$\frac{\mathrm{d}}{\mathrm{d}x}(u+v)=\frac{\mathrm{d}u}{\mathrm{d}x}+\frac{\mathrm{d}v}{\mathrm{d}x}\qquad\text{(MB1.4a)}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}uv=u\frac{\mathrm{d}v}{\mathrm{d}x}+v\frac{\mathrm{d}u}{\mathrm{d}x}\qquad\text{(MB1.4b)}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{u}{v}=\frac{1}{v}\frac{\mathrm{d}u}{\mathrm{d}x}-\frac{u}{v^2}\frac{\mathrm{d}v}{\mathrm{d}x}\qquad\text{(MB1.4c)}$$

Brief illustration MB1.2 Derivatives

To differentiate the function $f=\sin^2 ax/x^2$ use eqn MB1.4 to write

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\sin^2 ax}{x^2}=\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\sin ax}{x}\right)\left(\frac{\sin ax}{x}\right)=2\left(\frac{\sin ax}{x}\right)\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\sin ax}{x}\right)$$
$$=2\left(\frac{\sin ax}{x}\right)\left\{\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\sin ax+\sin ax\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{x}\right\}$$
$$=2\left\{\frac{a}{x^2}\sin ax\cos ax-\frac{\sin^2 ax}{x^3}\right\}$$

The function and this first derivative are plotted in Fig. MB1.2.

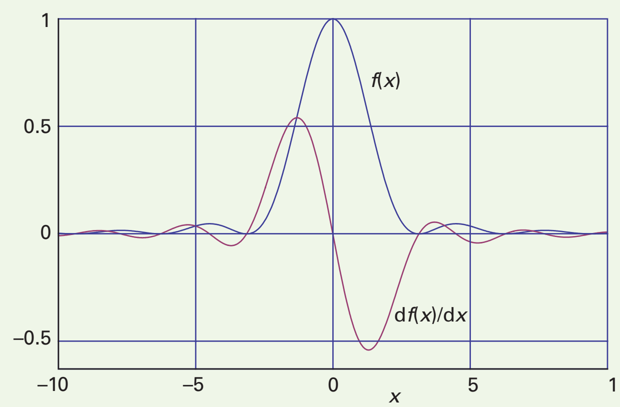

Figure MB1.2 The function considered in *Brief illustration* MB1.2 and its first derivative.

MB1.3 Series expansions

One application of differentiation is to the development of power series for functions. The **Taylor series** for a function $f(x)$ in the vicinity of $x=a$ is

$$f(x)=f(a)+\left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)_a(x-a)+\frac{1}{2!}\left(\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right)_a(x-a)^2+\cdots$$
$$=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{\mathrm{d}^n f}{\mathrm{d}x^n}\right)_a(x-a)^n \qquad \text{Taylor series} \qquad \text{(MB1.5)}$$

where the notation $(\ldots)_a$ means that the derivative is evaluated at $x=a$ and $n!$ denotes a **factorial** given by

$$n!=n(n-1)(n-2)\ldots1,\quad 0!=1 \qquad \text{Factorial} \qquad \text{(MB1.6)}$$

The **Maclaurin series** for a function is a special case of the Taylor series in which $a=0$.

Brief illustration MB1.3 Series expansion

To evaluate the expansion of $\cos x$ around $x=0$ we note that

$$\left(\frac{\mathrm{d}}{\mathrm{d}x}\cos x\right)_0=(-\sin x)_0=0 \qquad \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\cos x\right)_0=(-\cos x)_0=-1$$

and in general

$$\left(\frac{\mathrm{d}^n}{\mathrm{d}x^n}\cos x\right)_0=\begin{cases}0 \text{ for } n \text{ odd}\\(-1)^{n/2} \text{ for } n \text{ even}\end{cases}$$

Therefore,

$$\cos x=\sum_{n\text{ even}}^{\infty}\frac{(-1)^{n/2}}{n!}x^n=1-\tfrac{1}{2}x^2+\tfrac{1}{24}x^4-\cdots$$

The following Taylor series (specifically, Maclaurin series) are used at various stages in the text:

$$(1+x)^{-1}=1-x+x^2-\cdots=\sum_{n=0}^{\infty}(-1)^n x^n \qquad \text{(MB1.7a)}$$

$$\mathrm{e}^x=1+x+\tfrac{1}{2}x^2+\cdots=\sum_{n=0}^{\infty}\frac{x^n}{n!} \qquad \text{(MB1.7b)}$$

$$\ln(1+x)=x-\tfrac{1}{2}x^2+\tfrac{1}{3}x^3-\cdots=\sum_{n=1}^{\infty}(-1)^{n+1}\frac{x^n}{n} \qquad \text{(MB1.7c)}$$

Taylor series are used to simplify calculations, for when $x\ll1$ it is possible, to a good approximation, to terminate the series after one or two terms. Thus, provided $x\ll1$ we can write

$$(1+x)^{-1}\approx1-x \qquad \text{(MB1.8a)}$$

$$\mathrm{e}^x\approx1+x \qquad \text{(MB1.8b)}$$

$$\ln(1+x)\approx x \qquad \text{(MB1.8c)}$$

A series is said to **converge** if the sum approaches a finite, definite value as n approaches infinity. If the sum does not approach a finite, definite value, then the series is said to **diverge**. Thus, the series in eqn MB1.7a converges for $x<1$ and diverges for $x\geq1$.There are a variety of tests for convergence, which are explained in mathematics texts.

MB1.4 Integration: definitions

Integration (which formally is the inverse of differentiation) is concerned with the areas under curves. The **integral** of a

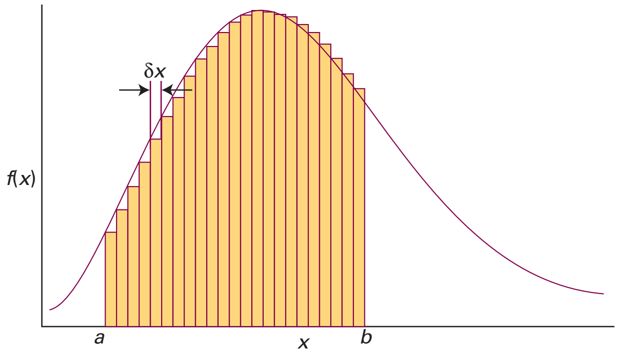

Figure MB1.3 A definite integral is evaluated by forming the product of the value of the function at each point and the increment δx, with $\delta x \to 0$, and then summing the products $f(x)\delta x$ for all values of x between the limits a and b. It follows that the value of the integral is the area under the curve between the two limits.

function $f(x)$, which is denoted $\int f\,dx$ (the symbol $\int$ is an elongated S denoting a sum), between the two values $x=a$ and $x=b$ is defined by imagining the x axis as divided into strips of width δx and evaluating the following sum:

$$\int_a^b f(x)dx = \lim_{\delta x \to 0} \sum_i f(x_i)\delta x$$ *Definition* Integration (MB1.9)

As can be appreciated from Fig. MB1.3, the integral is the area under the curve between the limits a and b. The function to be integrated is called the **integrand**. It is an astonishing mathematical fact that the integral of a function is the inverse of the differential of that function in the sense that if we differentiate f and then integrate the resulting function, then we obtain the original function f (to within a constant). The function in eqn MB1.9 with the limits specified is called a **definite integral**. If it is written without the limits specified, then we have an **indefinite integral**. If the result of carrying out an indefinite integration is $g(x)+C$, where C is a constant, the following notation is used to evaluate the corresponding definite integral:

$$I = \int_a^b f(x)dx = \{g(x)+C\}\Big|_a^b = \{g(b)+C\} - \{g(a)+C\}$$
$$= g(b) - g(a)$$ Definite integral (MB1.10)

Note that the constant of integration disappears. The definite and indefinite integrals encountered in this text are listed in the *Resource section*.

MB1.5 Integration: manipulations

When an indefinite integral is not in the form of one of those listed in the *Resource section* it is sometimes possible to transform it into one of the forms by using integration techniques such as:

Substitution. Introduce a variable u related to the independent variable x (for example, an algebraic relation such as $u=x^2-1$ or a trigonometric relation such as $u=\sin x$). Express the differential dx in terms of du (for these substitutions, $du=2x\,dx$ and $du=\cos x\,dx$, respectively). Then transform the original integral written in terms of x into an integral in terms of u upon which, in some cases, a standard form such as one of those listed in the *Resource section* can be used.

Brief illustration MB1.4 Integration by substitution

To evaluate the indefinite integral $\int \cos^2 x \sin x\,dx$ we make the substitution $u=\cos x$. It follows that $du/dx=-\sin x$, and therefore that $\sin x\,dx=-du$. The integral is therefore

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

To evaluate the corresponding definite integral, we have to convert the limits on x into limits on u. Thus, if the limits are $x=0$ and $x=\pi$, the limits become $u=\cos 0=1$ and $u=\cos \pi=-1$:

$$\int_0^\pi \cos^2 x \sin x\,dx = -\int_1^{-1} u^2\,du = \left\{-\tfrac{1}{3}u^3 + C\right\}\Big|_1^{-1} = \frac{2}{3}$$

Integration by parts. For two functions $f(x)$ and $g(x)$:

$$\int f\frac{dg}{dx}dx = fg - \int g\frac{df}{dx}dx$$ Integration by parts (MB1.11a)

which may be abbreviated as:

$$\int f dg = fg - \int g df$$ (MB1.11b)

Brief illustration MB1.5 Integration by parts

Integrals over xe^{-ax} and their analogues occur commonly in the discussion of atomic structure and spectra. They may be integrated by parts, as in the following:

$$\int_0^\infty \overset{f}{x}\,\overbrace{e^{-ax}}^{dg/dx}\,dx = \overset{f}{x}\,\overbrace{\frac{e^{-ax}}{-a}}^{g}\Bigg|_0^\infty - \int_0^\infty \overbrace{\frac{e^{-ax}}{-a}}^{g}\,\overset{df/dx}{1}\,dx$$
$$= -\frac{xe^{-ax}}{a}\Bigg|_0^\infty + \frac{1}{a}\int_0^\infty e^{-ax}\,dx = 0 - \frac{e^{-ax}}{a^2}\Bigg|_0^\infty$$
$$= \frac{1}{a^2}$$

MB1.6 Multiple integrals

A function may depend on more than one variable, in which case we may need to integrate over both the variables:

$$I=\int_a^b\int_c^d f(x,y)\mathrm{d}x\mathrm{d}y \qquad \text{(MB1.12)}$$

We (but not everyone) adopt the convention that a and b are the limits of the variable x and c and d are the limits for y (as depicted by the colours in this instance). This procedure is simple if the function is a product of functions of each variable and of the form $f(x,y)=X(x)Y(y)$. In this case, the double integral is just a product of each integral:

$$I=\int_a^b\int_c^d X(x)Y(y)\mathrm{d}x\mathrm{d}y=\int_a^b X(x)\mathrm{d}x\int_c^d Y(y)\mathrm{d}y \qquad \text{(MB1.13)}$$

Brief illustration MB1.6 A double integral

Double integrals of the form

$$I=\int_0^{L_1}\int_0^{L_2}\sin^2(\pi x/L_1)\sin^2(\pi y/L_2)\mathrm{d}x\mathrm{d}y$$

occur in the discussion of the translational motion of a particle in two dimensions, where L_1 and L_2 are the maximum extents of travel along the x- and y-axes, respectively. To evaluate I we use eqn MB1.13 and an integral listed in the *Resource section* to write

$$\begin{aligned}I &\overset{\text{Integral T.2}}{=} \int_0^{L_1}\sin^2(\pi x/L_1)\mathrm{d}x\int_0^{L_2}\sin^2(\pi y/L_2)\mathrm{d}y\\ &=\left\{\tfrac{1}{2}x-\frac{\sin(2\pi x/L_1)}{4\pi/L_1}+C\right\}\Bigg|_0^{L_1}\left\{\tfrac{1}{2}y-\frac{\sin(2\pi y/L_2)}{4\pi/L_2}+C\right\}\Bigg|_0^{L_2}\\ &=\tfrac{1}{4}L_1L_2\end{aligned}$$

PART 1 Common integrals

Algebraic functions

A.1 $\int x^n \,dx = \frac{x^{n+1}}{n+1} + \text{constant}, \; n \neq -1$

A.2 $\int \frac{1}{x} \,dx = \ln x + \text{constant}$

Exponential functions

E.1 $\int_0^\infty x^n e^{-ax} \,dx = \frac{n!}{a^{n+1}}, \quad n! = n(n-1)\ldots 1; \; 0! \equiv 1$

E.2 $\int_0^\infty \frac{x^4 e^x}{(e^x-1)^2} \,dx = \frac{\pi^4}{15}$

Gaussian functions

G.1 $\int_0^\infty e^{-ax^2} \,dx = \frac{1}{2}\left(\frac{\pi}{a}\right)^{1/2}$

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

G.3 $\int_0^\infty x^2 e^{-ax^2} \,dx = \frac{1}{4}\left(\frac{\pi}{a^3}\right)^{1/2}$

G.4 $\int_0^\infty x^3 e^{-ax^2} \,dx = \frac{1}{2a^2}$

G.5 $\int_0^\infty x^4 e^{-ax^2} \,dx = \frac{3}{8a^2}\left(\frac{\pi}{a}\right)^{1/2}$

G.6 $\operatorname{erf} z = \frac{2}{\pi^{1/2}} \int_0^z e^{-x^2} \,dx \qquad \operatorname{erfc} z = 1 - \operatorname{erf} z$

G.7 $\int_0^\infty x^{2m+1} e^{-ax^2} \,dx = \frac{m!}{2a^{m+1}}$

G.8 $\int_0^\infty x^{2m} e^{-ax^2} \,dx = \frac{(2m-1)!!}{2^{m+1} a^m}\left(\frac{\pi}{a}\right)^{1/2}$

$(2m-1)!! = 1 \times 3 \times 5 \cdots \times (2m-1)$

Trigonometric functions

T.1 $\int \sin ax \,dx = -\frac{1}{a}\cos ax + \text{constant}$

T.2 $\int \sin^2 ax \,dx = \frac{1}{2}x - \frac{\sin 2ax}{4a} + \text{constant}$

T.3 $\int \sin^3 ax \,dx = -\frac{(\sin^2 ax + 2)\cos ax}{3a} + \text{constant}$

T.4 $\int \sin^4 ax \,dx = \frac{3x}{8} - \frac{3}{8a}\sin ax \cos ax - \frac{1}{4a}\sin^3 ax \cos ax + \text{constant}$

T.5 $\int \sin ax \sin bx \,dx = \frac{\sin(a-b)x}{2(a-b)} - \frac{\sin(a+b)x}{2(a+b)} + \text{constant}, \; a^2 \neq b^2$

T.6 $\int_0^L \sin nax \sin^2 ax \,dx = -\frac{1}{2a}\left\{\frac{1}{n} - \frac{1}{2(n+2)} - \frac{1}{2(n-2)}\right\} \times \{(-1)^n - 1\}$

T.7 $\int \sin ax \cos ax \,dx = \frac{1}{2a}\sin^2 ax + \text{constant}$

T.8 $\int \sin bx \cos ax \,dx = \frac{\cos(a-b)x}{2(a-b)} - \frac{\cos(a+b)x}{2(a+b)} + \text{constant}, \; a^2 \neq b^2$

T.9 $\int x \sin ax \sin bx \,dx = -\frac{d}{da}\int \sin bx \cos ax \,dx$

T.10 $\int \cos^2 ax \sin ax \,dx = -\frac{1}{3a}\cos^3 ax + \text{constant}$

T.11 $\int x \sin^2 ax \,dx = \frac{x^2}{4} - \frac{x \sin 2ax}{4a} - \frac{\cos 2ax}{8a^2} + \text{constant}$

T.12 $\int x^2 \sin^2 ax \,dx = \frac{x^3}{6} - \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right)\sin 2ax - \frac{x \cos 2ax}{4a^2} + \text{constant}$

T.13 $\int x \cos ax \,dx = \frac{1}{a^2}\cos ax + \frac{x}{a}\sin ax + \text{constant}$

Mathematical background 3 Complex numbers

We describe here general properties of complex numbers and functions, which are mathematical constructs frequently encountered in quantum mechanics.

MB3.1 Definitions

Complex numbers have the general form

$$z = x + \mathrm{i}y \quad \text{General form of a complex number} \quad \text{(MB3.1)}$$

where $\mathrm{i}=(-1)^{1/2}$. The real numbers x and y are, respectively, the real and imaginary parts of z, denoted Re(z) and Im(z). When $y=0$, $z=x$ is a real number; when $x=0$, $z=\mathrm{i}y$ is a pure imaginary number. Two complex numbers $z_1=x_1+\mathrm{i}y_1$ and $z_2=x_2+\mathrm{i}y_2$ are equal when $x_1=x_2$ and $y_1=y_2$. Although the general form of the imaginary part of a complex number is written iy, a specific numerical value is typically written in the reverse order; for instance, as 3i.

The **complex conjugate** of z, denoted z^*, is formed by replacing i by –i:

$$z^* = x - \mathrm{i}y \quad \text{Complex conjugate} \quad \text{(MB3.2)}$$

The product of z^* and z is denoted $|z|^2$ and is called the **square modulus** of z. From eqns MB3.1 and MB3.2,

$$|z|^2 = (x+\mathrm{i}y)(x-\mathrm{i}y) = x^2 + y^2 \quad \text{Square modulus} \quad \text{(MB3.3)}$$

since $\mathrm{i}^2=-1$. The square modulus is a real number. The **absolute value** or **modulus** is itself denoted $|z|$ and is given by:

$$|z| = (z^*z)^{1/2} = (x^2+y^2)^{1/2} \quad \text{Absolute value or modulus} \quad \text{(MB3.4)}$$

Since $zz^*=|z|^2$ it follows that $z\times(z^*/|z|^2)=1$, from which we can identify the (multiplicative) **inverse** of z (which exists for all nonzero complex numbers):

$$z^{-1} = \frac{z^*}{|z|^2} \quad \text{Inverse of a complex number} \quad \text{(MB3.5)}$$

Brief illustration MB3.1 Inverse

Consider the complex number $z=8-3\mathrm{i}$. Its square modulus is

$$|z|^2 = z^*z = (8-3\mathrm{i})^*(8-3\mathrm{i}) = (8+3\mathrm{i})(8-3\mathrm{i}) = 64+9 = 73$$

The modulus is therefore $|z|=73^{1/2}$. From eqn MB3.5, the inverse of z is

$$z^{-1} = \frac{8+3\mathrm{i}}{73} = \frac{8}{73} + \frac{3}{73}\mathrm{i}$$

MB3.2 Polar representation

The complex number $z=x+\mathrm{i}y$ can be represented as a point in a plane, the **complex plane**, with Re(z) along the x-axis and Im(z) along the y-axis (Fig. MB3.1). If, as shown in the figure, r and ϕ denote the polar coordinates of the point, then since $x=r\cos\phi$ and $y=r\sin\phi$, we can express the complex number in **polar form** as

$$z = r(\cos\phi + \mathrm{i}\sin\phi) \quad \text{Polar form of a complex number} \quad \text{(MB3.6)}$$

The angle ϕ, called the **argument** of z, is the angle that z makes with the x-axis. Because $y/x=\tan\phi$, it follows that the polar form can be constructed from

$$r = (x^2+y^2)^{1/2} = |z| \qquad \phi = \arctan\frac{y}{x} \quad \text{(MB3.7a)}$$

To convert from polar to Cartesian form, use

$$x = r\cos\phi \text{ and } y = r\sin\phi \text{ to form } z = x+\mathrm{i}y \quad \text{(MB3.7b)}$$

One of the most useful relations involving complex numbers is **Euler's formula**:

$$\mathrm{e}^{\mathrm{i}\phi} = \cos\phi + \mathrm{i}\sin\phi \quad \text{Euler's formula} \quad \text{(MB3.8a)}$$

The simplest proof of this relation is to expand the exponential function as a power series and to collect real and imaginary terms. It follows that

$$\cos\phi = \tfrac{1}{2}(\mathrm{e}^{\mathrm{i}\phi}+\mathrm{e}^{-\mathrm{i}\phi}) \qquad \sin\phi = -\tfrac{1}{2}\mathrm{i}(\mathrm{e}^{\mathrm{i}\phi}-\mathrm{e}^{-\mathrm{i}\phi}) \quad \text{(MB3.8b)}$$

The polar form in eqn MB3.6 then becomes

$$z = r\mathrm{e}^{\mathrm{i}\phi} \quad \text{(MB3.9)}$$

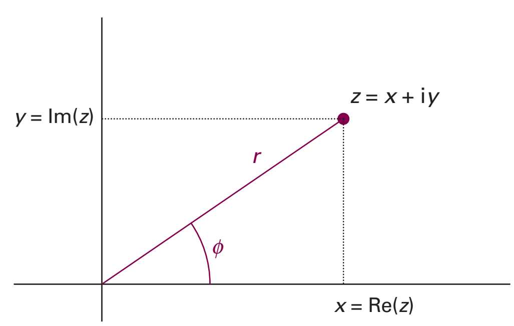

Figure MB3.1 The representation of a complex number z as a point in the complex plane using Cartesian coordinates (x,y) or polar coordinates (r,ϕ).

Brief illustration MB3.2 Polar representation

Consider the complex number $z = 8 - 3i$. From *Brief illustration* MB3.1, $r = |z| = 73^{1/2}$. The argument of z is

$$\theta = \arctan\left(\frac{-3}{8}\right) = -0.359\,\text{rad, or } -20.6°$$

The polar form of the number is therefore

$$z = 73^{1/2} e^{-0.359i}$$

MB3.3 Operations

The following rules apply for arithmetic operations for the complex numbers $z_1 = x_1 + iy_1$ and $z_2 = x_2 + iy_2$.

1. Addition: $z_1 + z_2 = (x_1 + x_2) + i(y_1 + y_2)$ (MB3.10a)
2. Subtraction: $z_1 - z_2 = (x_1 - x_2) + i(y_1 - y_2)$ (MB3.10b)
3. Multiplication:

$$\begin{aligned} z_1 z_2 &= (x_1 + iy_1)(x_2 + iy_2) \\ &= (x_1 x_2 - y_1 y_2) + i(x_1 y_2 + y_1 x_2) \end{aligned} \quad \text{(MB3.10c)}$$

4. Division: We interpret z_1/z_2 as $z_1 z_2^{-1}$ and use eqn MB3.5 for the inverse:

$$\frac{z_1}{z_2} = z_1 z_2^{-1} = \frac{z_1 z_2^*}{|z_2|^2} \quad \text{(MB3.10d)}$$

Brief illustration MB3.3 Operations with numbers

Consider the complex numbers $z_1 = 6 + 2i$ and $z_2 = -4 - 3i$. Then

$$z_1 + z_2 = (6 - 4) + (2 - 3)i = 2 - i$$

$$z_1 - z_2 = 10 + 5i$$

$$z_1 z_2 = \{6(-4) - 2(-3)\} + \{6(-3) + 2(-4)\}i = -18 - 26i$$

$$\frac{z_1}{z_2} = (6 + 2i)\left(\frac{-4 + 3i}{25}\right) = -\frac{6}{5} + \frac{2}{5}i$$

The polar form of a complex number is commonly used to perform arithmetical operations. For instance the product of two complex numbers in polar form is

$$z_1 z_2 = (r_1 e^{i\phi_1})(r_2 e^{i\phi_2}) = r_1 r_2 e^{i(\phi_1 + \phi_2)} \quad \text{(MB3.11)}$$

This multiplication can be depicted in the complex plane, as shown in Fig. MB3.2.

The nth power and the nth root of a complex number are

$$z^n = (re^{i\phi})^n = r^n e^{in\phi} \qquad z^{1/n} = (re^{i\phi})^{1/n} = r^{1/n} e^{i\phi/n} \quad \text{(MB3.12)}$$

The depictions in the complex plane are shown in Fig. MB3.3.

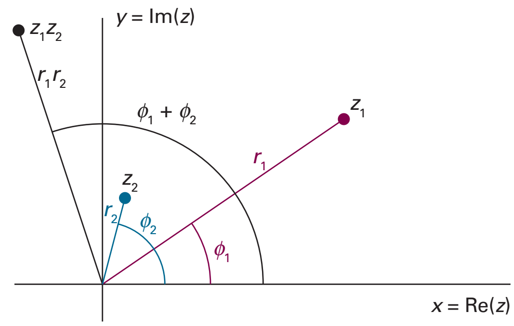

Figure MB3.2 The multiplication of two complex numbers depicted in the complex plane.

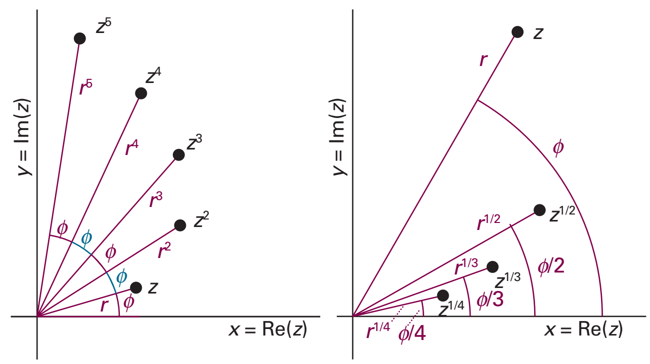

Figure MB3.3 The nth powers ($n = 1, 2, 3, 4, 5$) and the nth roots ($n = 1, 2, 3, 4$) of a complex number depicted in the complex plane.

Brief illustration MB3.4 Roots

To determine the 5th root of $z = 8 - 3i$, we note that from *Brief illustration* MB3.2 its polar form is

$$z = 73^{1/2} e^{-0.359i} = 8.544 e^{-0.359i}$$

The 5th root is therefore

$$z^{1/5} = (8.544 e^{-0.359i})^{1/5} = 8.544^{1/5} e^{-0.359i/5} = 1.536 e^{-0.0718i}$$

It follows that $x = 1.536 \cos(-0.0718) = 1.532$ and $y = 1.536 \sin(-0.0718) = -0.110$ (note that we work in radians), so

$$(8 - 3i)^{1/5} = 1.532 - 0.110i$$

Mathematical background 4 Differential equations

A **differential equation** is a relation between a function and its derivatives, as in

$$a\frac{d^2f}{dx^2}+b\frac{df}{dx}+cf=0 \qquad \text{(MB4.1)}$$

where f is a function of the variable x and the factors a, b, c may be either constants or functions of x. If the unknown function depends on only one variable, as in this example, the equation is called an **ordinary differential equation**; if it depends on more than one variable, as in

$$a\frac{\partial^2f}{\partial x^2}+b\frac{\partial^2f}{\partial y^2}+cf=0 \qquad \text{(MB4.2)}$$

it is called a **partial differential equation**. Here, f is a function of x and y, and the factors a, b, c may be either constants or functions of both variables. Note the change in symbol from d to ∂ to signify a *partial derivative* (see *Mathematical background* 2).

MB4.1 The structure of differential equations

The **order** of the differential equation is the order of the highest derivative that occurs in it: both examples above are second-order equations. Only rarely in science is a differential equation of order higher than two encountered.

A **linear differential equation** is one for which if f is a solution then so is constant×f. Both examples above are linear. If the 0 on the right were replaced by a different number or a function other than f, then they would cease to be linear.

Solving a differential equation means something different from solving an algebraic equation. In the latter case, the solution is a value of the variable x (as in the solution $x=2$ of the quadratic equation $x^2-4=0$). The solution of a differential equation is the entire function that satisfies the equation, as in

$$\frac{d^2f}{dx^2}+f=0, \quad f(x)=A\sin x+B\cos x \qquad \text{(MB4.3)}$$

with A and B constants. The process of finding a solution of a differential equation is called **integrating** the equation. The solution in eqn MB4.3 is an example of a **general solution** of a differential equation; that is, it is the most general solution of the equation and is expressed in terms of a number of constants (A and B in this case). When the constants are chosen to accord with certain specified **initial conditions** (if one variable is the time) or certain **boundary conditions** (to fulfil certain spatial restrictions on the solutions), we obtain the **particular solution** of the equation. The particular solution of a first-order differential equation requires one such condition; a second-order differential equation requires two.

Brief illustration MB4.1 Particular solutions

If we are informed that $f(0)=0$, then because from eqn MB4.3 it follows that $f(0)=B$, we can conclude that $B=0$. That still leaves A undetermined. If we are also told that $df/dx=2$ at $x=0$ (that is, $f'(0)=2$, where the prime denotes a first derivative), then because the general solution (but with $B=0$) implies that $f'(x)=A\cos x$, we know that $f'(0)=A$, and therefore $A=2$. The particular solution is therefore $f(x)=2\sin x$. Figure MB4.1 shows a series of particular solutions corresponding to different boundary conditions.

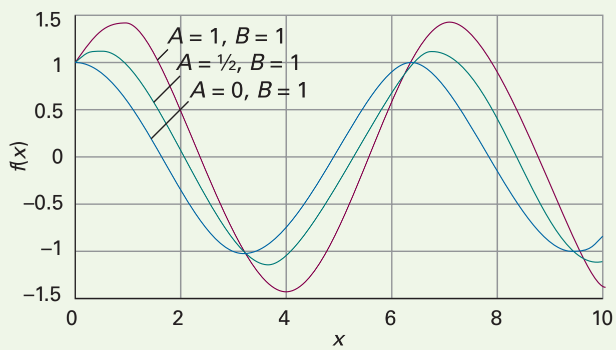

Figure MB4.1 The solution of the differential equation in *Brief illustration* MB4.1 with three different boundary conditions (as indicated by the resulting values of the constants A and B).

MB4.2 The solution of ordinary differential equations

The first-order linear differential equation

$$\frac{df}{dx}+af=0 \qquad \text{(MB4.4a)}$$

with a a function of x or a constant can be solved by direct integration. To proceed, we use the fact that the quantities df and dx (called *differentials*) can be treated algebraically like any quantity and rearrange the equation into

$$\frac{df}{f}=-a\,dx \qquad \text{(MB4.4b)}$$

and integrate both sides. For the left-hand side, we use the familiar result $\int dy/y=\ln y+\text{constant}$. After pooling all the constants into a single constant C, we obtain:

$$\ln f(x)=-\int a\,dx+C \qquad \text{(MB4.4c)}$$

Brief illustration MB4.2 The solution of a first-order equation

Suppose that in eqn MB4.4a the factor $a=2x$; then the general solution, eqn MB4.4c, is

$$\ln f(x)=-2\int x\,dx+C=-x^2+C$$

(We have absorbed the constant of integration into the constant C.) Therefore

$$f(x)=Ne^{-x^2}, \quad N=e^C$$

If we are told that $f(0)=1$, then we can infer that $N=1$ and therefore that $f(x)=e^{-x^2}$.

Even the solutions of first-order differential equations quickly become more complicated. A nonlinear first-order equation of the form

$$\frac{df}{dx}+af=b \qquad \text{(MB4.5a)}$$

with a and b functions of x (or constants) has a solution of the form

$$f(x)e^{\int a\,dx}=\int e^{\int a\,dx}b\,dx+C \qquad \text{(MB4.5b)}$$

as may be verified by differentiation. Mathematical software packages can often perform the required integrations.

Second-order differential equations are in general much more difficult to solve than first-order equations. One powerful approach commonly used to lay siege to second-order differential equations is to express the solution as a power series:

$$f(x)=\sum_{n=0}^{\infty}c_n x^n \qquad \text{(MB4.6)}$$

and then to use the differential equation to find a relation between the coefficients. This approach results, for instance, in the Hermite polynomials that form part of the solution of the Schrödinger equation for the harmonic oscillator (Topic 8B). Many of the second-order differential equations that occur in this text are tabulated in compilations of solutions or can be solved with mathematical software, and the specialized techniques that are needed to establish the form of the solutions may be found in mathematical texts.

MB4.3 The solution of partial differential equations

The only partial differential equations that we need to solve are those that can be separated into two or more ordinary differential equations by the technique known as **separation of variables**. To discover if the differential equation in eqn MB4.2 can be solved by this method we suppose that the full solution can be factored into functions that depend only on x or only on y, and write $f(x,y)=X(x)Y(y)$. At this stage there is no guarantee that the solution can be written in this way. Substituting this trial solution into the equation and recognizing that

$$\frac{\partial^2 XY}{\partial x^2}=Y\frac{d^2X}{dx^2} \qquad \frac{\partial^2 XY}{\partial y^2}=X\frac{d^2Y}{dy^2}$$

we obtain

$$aY\frac{d^2X}{dx^2}+bX\frac{d^2Y}{dy^2}+cXY=0$$

We are using d instead of ∂ at this stage to denote differentials because each of the functions X and Y depends on one variable, x and y, respectively. Division through by XY turns this equation into

$$\frac{a}{X}\frac{d^2X}{dx^2}+\frac{b}{Y}\frac{d^2Y}{dy^2}+c=0$$

Now suppose that a is a function only of x, b a function of y, and c a constant. (There are various other possibilities that permit the argument to continue.) Then the first term depends only on x and the second only on y. If x is varied, only the first term can change. But as the other two terms do not change and the sum of the three terms is a constant (0), even that first term must be a constant. The same is true of the second term. Therefore because each term is equal to a constant, we can write

$$\frac{a}{X}\frac{d^2X}{dx^2}=c_1 \qquad \frac{b}{Y}\frac{d^2Y}{dy^2}=c_2 \qquad \text{with } c_1+c_2=-c$$

We now have two ordinary differential equations to solve by the techniques described in Section MB4.2. An example of this procedure is given in Topic 8A, for a particle in a two-dimensional region.