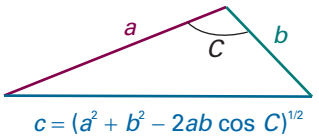

Fig. A2.4 The graphical representation of the law of cosines.

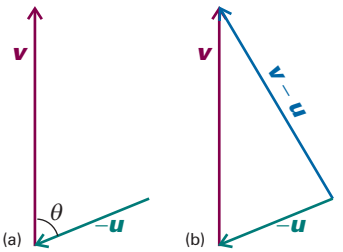

Fig. A2.5 The graphical method for subtraction of the vector $\boldsymbol{u}$ from the vector $\boldsymbol{v}$ (as shown in Fig. A2.2a) consists of two steps: (a) reversing the direction of $\boldsymbol{u}$ to form $-\boldsymbol{u}$, and (b) adding $-\boldsymbol{u}$ to $\boldsymbol{v}$.

$$v_{\text{res}}^2 = v^2 + u^2 - 2vu\cos(180° - \theta)$$

Because $\cos(180° - \theta) = -\cos\theta$, it follows after taking the square-root of both sides of the preceding expression that

$$v_{\text{res}} = (v^2 + u^2 + 2vu\cos\theta)^{1/2} \tag{A2.20}$$

The subtraction of vectors follows the same principles outlined above for addition. Consider again the vectors shown in Fig. A2.2a. We note that subtraction of $\boldsymbol{u}$ from $\boldsymbol{v}$ amounts to addition of $-\boldsymbol{u}$ to $\boldsymbol{v}$. It follows that in the first step of subtraction we draw $-\boldsymbol{u}$ by reversing the direction of $\boldsymbol{u}$ (Fig. A2.5a) Then, the second step consists of adding the $-\boldsymbol{u}$ to $\boldsymbol{v}$ by using the strategy shown in Fig. A2.2c: we draw a resultant vector $\boldsymbol{v}_{\text{res}}$ by joining the tail of $-\boldsymbol{u}$ to the head of $\boldsymbol{v}$.

2 Multiplication. There are two ways to multiply vectors. In one procedure, the **cross-product** of two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ is a vector defined as

$$\boldsymbol{u}\times\boldsymbol{v} = (uv\sin\theta)\boldsymbol{l} \tag{A2.21a}$$

where θ is the angle between the two vectors and $\boldsymbol{l}$ is a unit vector perpendicular to both $\boldsymbol{u}$ and $\boldsymbol{v}$, with a direction determined as in Fig. A2.6. An equivalent definition is

$$\boldsymbol{u}\times\boldsymbol{v} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ u_x & u_y & u_z \\ v_x & v_y & v_z \end{vmatrix} = (u_y v_z - u_z v_y)\boldsymbol{i} - (u_x v_z - u_z v_x)\boldsymbol{j} + (u_x v_y - u_y v_x)\boldsymbol{k} \tag{A2.21b}$$

where the structure in the middle is a determinant (see below). The second type of vector multiplication is the **scalar product** (or **dot product**) of two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$:

$$\boldsymbol{u}\cdot\boldsymbol{v} = uv\cos\theta \tag{A2.22}$$

As its name suggests, the scalar product of two vectors is a scalar.

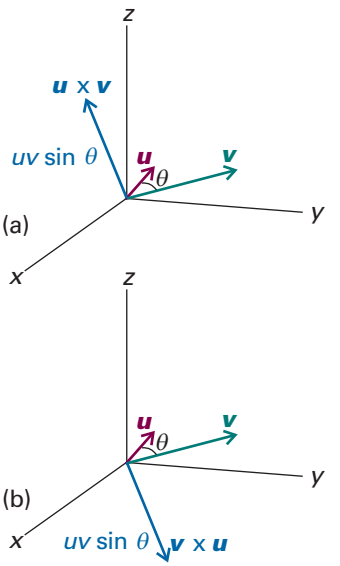

Fig. A2.6 The direction of the cross-products of two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ with an angle θ between them: (a) $\boldsymbol{u}\times\boldsymbol{v}$ and (b) $\boldsymbol{v}\times\boldsymbol{u}$. Note that the cross-product, and the unit vector $\boldsymbol{l}$ of eqn A2.21, are perpendicular to both $\boldsymbol{u}$ and $\boldsymbol{v}$ but the direction depends on the order in which the product is taken.

Calculus

A2.4 Differentiation and integration

Rates of change of functions—slopes of their graphs—are best discussed in terms of the infinitesimal calculus. The slope of a function, like the slope of a hill, is obtained by dividing the rise of the hill by the horizontal distance (Fig. A2.7). However, because

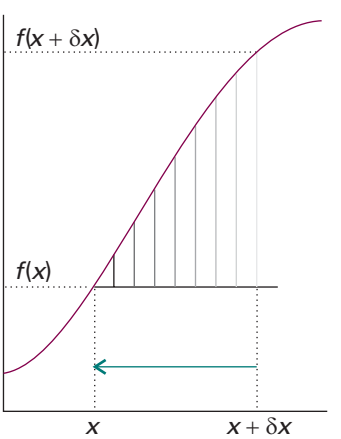

Fig. A2.7 The slope of $f(x)$ at x, $\mathrm{d}f/\mathrm{d}x$, is obtained by making a series of approximations to the value of $f(x+\delta x) - f(x)$ divided by the change in x, denoted δx, and allowing δx to approach 0 (as indicated by the vertical lines getting closer to x.

the slope may vary from point to point, we should make the horizontal distance between the points as small as possible. In fact, we let it become infinitesimally small —hence the name *infinitesimal* calculus. The values of a function f at two locations x and $x+\delta x$ are $f(x)$ and $f(x+\delta x)$, respectively. Therefore, the slope of the function f at x is the vertical distance, which we write δf, divided by the horizontal distance, which we write δx:

$$\text{Slope} = \frac{\text{rise in value}}{\text{horizontal distance}} = \frac{\delta f}{\delta x} = \frac{f(x+\delta x)-f(x)}{\delta x} \tag{A2.23}$$

The slope at x itself is obtained by letting the horizontal distance become zero, which we write $\lim \delta x \to 0$. In this limit, the δ is replaced by a d, and we write

$$\text{Slope at } x = \frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{\delta x \to 0} \frac{f(x+\delta x)-f(x)}{\delta x} \tag{A2.24}$$

To work out the slope of any function, we work out the expression on the right: this process is called **differentiation** and the expression for $\mathrm{d}f/\mathrm{d}x$ is the **derivative** of the function f with respect to the variable x. Some important derivatives are given inside the front cover of the text. Most of the functions encountered in chemistry can be differentiated by using the following rules (noting that in these expressions, derivatives $\mathrm{d}f/\mathrm{d}x$ are written as $\mathrm{d}f$):

Rule 1 For two functions f and g:

$$\mathrm{d}(f+g) = \mathrm{d}f + \mathrm{d}g \tag{A2.25}$$

Rule 2 (the product rule) For two functions f and g:

$$\mathrm{d}(fg) = f\,\mathrm{d}g + g\,\mathrm{d}f \tag{A2.26}$$

Rule 3 (the quotient rule) For two functions f and g:

$$\mathrm{d}\frac{f}{g} = \frac{1}{g}\mathrm{d}f - \frac{f}{g^2}\mathrm{d}g \tag{A2.27}$$

Rule 4 (the chain rule) For a function $f = f(g)$, where $g = g(t)$,

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\mathrm{d}f}{\mathrm{d}g}\frac{\mathrm{d}g}{\mathrm{d}t} \tag{A2.28}$$

The area under a graph of any function f is found by the techniques of **integration**. For instance, the area under the graph of the function f drawn in Fig. A2.8 can be written as the value of f evaluated at a point multiplied by the width of the region, δx, and then all those products $f(x)\delta x$ summed over all the regions:

$$\text{Area between } a \text{ and } b = \sum f(x)\delta x$$

When we allow δx to become infinitesimally small, written $\mathrm{d}x$, and sum an infinite number of strips, we write:

$$\text{Area between } a \text{ and } b = \int_a^b f(x)\mathrm{d}x \tag{A2.29}$$

The elongated S symbol on the right is called the **integral** of the function f. When written as $\int$ alone, it is the **indefinite integral** of the function. When written with limits (as in eqn A2.29), it is the **definite integral** of the function. The definite integral is the indefinite integral evaluated at the upper limit (b) minus the indefinite integral evaluated at the lower limit (a). The **average value** of a function $f(x)$ in the range $x = a$ to $x = b$ is

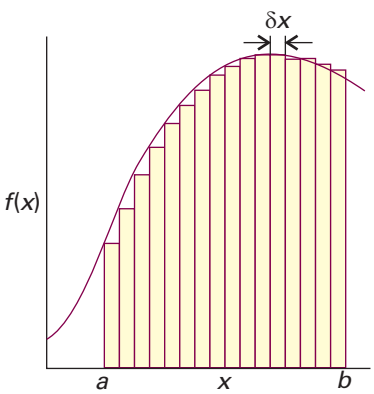

Fig. A2.8 The shaded area is equal to the definite integral of $f(x)$ between the limits a and b.

$$\text{Average value of } f(x) \text{ from } a \text{ to } b = \frac{1}{b-a}\int_a^b f(x)\mathrm{d}x \tag{A2.30}$$

The **mean value theorem** states that a continuous function has its mean value at least once in the range.

Integration is the inverse of differentiation. That is, if we integrate a function and then differentiate the result, we get back the original function. Some important integrals are given on the front back cover of the text. Many other standard forms are found in tables (see *Further reading*) and it is also possible to calculate definite and indefinite integrals with mathematical software. Two integration techniques are useful:

Technique 1 (integration by parts) For two functions f and g:

$$\int f\frac{\mathrm{d}g}{\mathrm{d}x}\mathrm{d}x = fg - \int g\frac{\mathrm{d}f}{\mathrm{d}x}\mathrm{d}x \tag{A2.31}$$

Technique 2 (method of partial fractions) To solve an integral of the form $\int \frac{1}{(a-x)(b-x)}\mathrm{d}x$, where a and b are constants, we write

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

and integrate the expression on the right. It follows that

$$\begin{aligned}\int \frac{\mathrm{d}x}{(a-x)(b-x)} &= \frac{1}{b-a}\left[\int\frac{\mathrm{d}x}{a-x} - \int\frac{\mathrm{d}x}{b-x}\right]\\ &= \frac{1}{b-a}\left(\ln\frac{1}{a-x} - \ln\frac{1}{b-x}\right) + \text{constant}\end{aligned} \tag{A2.32}$$

A2.5 Power series and Taylor expansions

A **power series** has the form

$$c_0 + c_1(x-a) + c_2(x-a)^2 + \cdots + c_n(x-a)^n + \cdots = \sum_{n=0}^{\infty} c_n(x-a)^n \tag{A2.33}$$

where c_n and a are constants. It is often useful to express a function $f(x)$ in the vicinity of $x = a$ as a special power series called the **Taylor series**, or **Taylor expansion**, which has the form:

$$\begin{aligned}f(x) &= f(a) + \left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)(x-a) + \frac{1}{2!}\left(\frac{\mathrm{d}^2f}{\mathrm{d}x^2}\right)_a(x-a)^2 + \cdots + \frac{1}{n!}\left(\frac{\mathrm{d}^nf}{\mathrm{d}x^n}\right)_a(x-a)^n\\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{\mathrm{d}^nf}{\mathrm{d}x^n}\right)_a(x-a)^n\end{aligned} \tag{A2.34}$$

where $n!$ denotes a **factorial**, given by

$$n! = n(n-1)(n-2)\ldots 1 \tag{A2.35}$$

By definition $0! = 1$. The following Taylor expansions are often useful:

$$\frac{1}{1+x} = 1 - x + x^2 + \cdots$$

$$\mathrm{e}^x = 1 + x + \tfrac{1}{2}x^2 + \cdots$$

$$\ln x = (x-1) - \tfrac{1}{2}(x-1)^2 + \tfrac{1}{3}(x-1)^3 - \tfrac{1}{4}(x-1)^4 + \cdots$$

$$\ln(1+x) = x - \tfrac{1}{2}x^2 + \tfrac{1}{3}x^3 - \cdots$$

If $x \ll 1$, then $(1+x)^{-1} \approx 1 - x$, $\mathrm{e}^x \approx 1 + x$, and $\ln(1+x) \approx x$.

A2.6 Partial derivatives

A **partial derivative** of a function of more than one variable, such as $f(x,y)$, is the slope of the function with respect to one of the variables, all the other variables being held constant (see Fig. 2.21). Although a partial derivative shows how a function changes when one variable changes, it may be used to determine how the function changes when more than one variable changes by an infinitesimal amount. Thus, if f is a function of x and y, then when x and y change by $\mathrm{d}x$ and $\mathrm{d}y$, respectively, f changes by

$$\mathrm{d}f = \left(\frac{\partial f}{\partial x}\right)_y \mathrm{d}x + \left(\frac{\partial f}{\partial y}\right)_x \mathrm{d}y \tag{A2.36}$$

where the symbol ∂ is used (instead of d) to denote a partial derivative. The quantity $\mathrm{d}f$ is also called the **differential** of f. For example, if $f = ax^3y + by^2$, then

$$\left(\frac{\partial f}{\partial x}\right)_y = 3ax^2y \qquad \left(\frac{\partial f}{\partial y}\right)_x = ax^3 + 2by$$

Then, when x and y undergo infinitesimal changes, f changes by

$$\mathrm{d}f = 3ax^2y\mathrm{d}x + (ax^3 + 2by)\mathrm{d}y$$

Partial derivatives may be taken in any order:

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x} \tag{A2.37}$$

For the function f given above, it is easy to verify that

$$\left(\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right)_y\right)_x = 3ax^2 \qquad \left(\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)_x\right)_y = 3ax^2$$

In the following, z is a variable on which x and y depend (for example, x, y, and z might correspond to p, V, and T).

Relation 1 When x is changed at constant z:

$$\left(\frac{\partial f}{\partial x}\right)_z = \left(\frac{\partial f}{\partial x}\right)_y + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial x}\right)_z \tag{A2.38}$$

Relation 2

$$\left(\frac{\partial y}{\partial x}\right)_z = \frac{1}{(\partial x/\partial y)_z} \tag{A2.39}$$

Relation 3

$$\left(\frac{\partial x}{\partial y}\right)_z = -\left(\frac{\partial x}{\partial z}\right)_y \left(\frac{\partial z}{\partial y}\right)_x \tag{A2.40}$$

By combining this relation and Relation 2 we obtain the **Euler chain relation**:

$$\left(\frac{\partial y}{\partial x}\right)_z \left(\frac{\partial x}{\partial z}\right)_y \left(\frac{\partial z}{\partial y}\right)_x = -1 \tag{A2.41}$$

Relation 4 This relation establishes whether or not $\mathrm{d}f$ is an **exact differential**.

$$\mathrm{d}f = g(x,y)\mathrm{d}x + h(x,y)\mathrm{d}y \qquad \text{is exact if} \quad \left(\frac{\partial g}{\partial y}\right)_x = \left(\frac{\partial h}{\partial x}\right)_y \tag{A2.42}$$

If $\mathrm{d}f$ is exact, its integral between specified limits is independent of the path.

A2.7 Functionals and functional derivatives

Just as a function f can be regarded as a set of mathematical procedures that associates a number $f(x)$ to a specified value of a variable x, so a **functional** G gives a prescription for associating a number $G[f]$ to a function $f(x)$ over a specified range of the variable x. That is, the functional is a function of a function. Functionals are important in quantum chemistry. We saw in Chapter 11 that the energy of a molecule is a functional of the electron density, which in turn is a function of the position.

To make the following discussion more concrete, consider the functional

$$G[f] = \int_0^1 f(x)^2 \, \mathrm{d}x \tag{A2.43}$$

If we let $f(x) = x$, then $G[f] = \frac{1}{3}$ over the range $0 \le x \le 1$. However, if $f(x) = \sin \pi x$, then $G[f] = \frac{1}{2}$ over the range $0 \le x \le 1$.

Just as the derivative of a function $f(x)$ tells us how the function changes with small changes δx in the variable x, so a **functional derivative** tells us about the variation δG of a functional $G[f]$ with small changes δf in the function $f(x)$. By analogy with eqn A2.24, we can write the following definition of the functional derivative as

$$\frac{\delta G}{\delta f} = \lim_{\delta f \to 0} \frac{G[f + \delta f] - G[f]}{\delta f} \tag{A2.44}$$

However, this equation does not give us a simple method for calculating the functional derivative. It can be shown that an alternative definition of $\delta G/\delta f$ is (see *Further reading*):

$$G[f + \delta f] - G[f] = \int_a^b \left(\frac{\delta G}{\delta f} \delta f(x) \right) \mathrm{d}x \tag{A2.45}$$

where the integral is evaluated in the range over which x varies.

To see how eqn A2.45 is used to calculate a functional derivative, consider the functional given by eqn A2.43. We begin by writing

$$\begin{aligned} G[f + \delta f] &= \int_0^1 \{f(x) + \delta f(x)\}^2 \mathrm{d}x = \int_0^1 \{f(x)^2 + 2f(x)\delta f(x) + \delta f(x)^2\} \mathrm{d}x \\ &= \int_0^1 \{f(x)^2 + 2f(x)\delta f(x)\} \mathrm{d}x = G[f] + \int_0^1 2f(x)\delta f(x) \mathrm{d}x \end{aligned}$$

where we have ignored the minute contribution from δf^2 to arrive at the penultimate expression and then used eqn A2.43 to write the final expression. It follows that

$$G[f + \delta f] - G[f] = \int_0^1 2f(x)\delta f(x) \mathrm{d}x$$

By comparing this expression with eqn A2.45, we see that the functional derivative is

$$\frac{\delta G}{\delta f} = 2f(x)$$

A2.8 Undetermined multipliers

Suppose we need to find the maximum (or minimum) value of some function f that depends on several variables $x_1, x_2, \ldots, x_n$. When the variables undergo a small change from x_i to $x_i + \delta x_i$ the function changes from f to $f + \delta f$, where

$$\delta f = \sum_i^n \left(\frac{\partial f}{\partial x_i}\right)\delta x_i \tag{A2.46}$$

At a minimum or maximum, $\delta f = 0$, so then

$$\sum_i^n \left(\frac{\partial f}{\partial x_i}\right)\delta x_i = 0 \tag{A2.47}$$

If the x_i were all independent, all the δx_i would be arbitrary, and this equation could be solved by setting each $(\partial f/\partial x_i) = 0$ individually. When the x_i are not all independent, the δx_i are not all independent, and the simple solution is no longer valid. We proceed as follows.

Let the constraint connecting the variables be an equation of the form $g = 0$. For example, in Chapter 16, one constraint was $n_0 + n_1 + \cdots = N$, which can be written

$$g = 0, \qquad \text{with} \quad g = (n_0 + n_1 + \cdots) - N$$

The constraint $g = 0$ is always valid, so g remains unchanged when the x_i are varied:

$$\delta g = \sum_i \left(\frac{\partial g}{\partial x_i}\right)\delta x_i = 0 \tag{A2.48}$$

Because δg is zero, we can multiply it by a parameter, λ, and add it to eqn A2.47:

$$\sum_i^n \left\{\left(\frac{\partial f}{\partial x_i}\right) + \lambda\left(\frac{\partial g}{\partial x_i}\right)\right\}\delta x_i = 0 \tag{A2.49}$$

This equation can be solved for one of the δx, δx_n for instance, in terms of all the other δx_i. All those other δx_i $(i = 1, 2, \ldots n-1)$ are independent, because there is only one constraint on the system. But here is the trick: λ is arbitrary; therefore we can choose it so that the coefficient of δx_n in eqn A2.49 is zero. That is, we choose λ so that

$$\left(\frac{\partial f}{\partial x_n}\right) + \lambda\left(\frac{\partial g}{\partial x_n}\right) = 0 \tag{A2.50}$$

Then eqn A2.49 becomes

$$\sum_i^{n-1} \left\{\left(\frac{\partial f}{\partial x_i}\right) + \lambda\left(\frac{\partial g}{\partial x_i}\right)\right\}\delta x_i = 0 \tag{A2.51}$$

Now the $n-1$ variations δx_i *are* independent, so the solution of this equation is

$$\left(\frac{\partial f}{\partial x_i}\right) + \lambda\left(\frac{\partial g}{\partial x_i}\right) = 0 \qquad i = 1, 2, \ldots, n-1 \tag{A2.52}$$

However, eqn A2.50 has exactly the same form as this equation, so the maximum or minimum of f can be found by solving

$$\left(\frac{\partial f}{\partial x_i}\right) + \lambda\left(\frac{\partial g}{\partial x_i}\right) = 0 \qquad i = 1, 2, \ldots, n \tag{A2.53}$$

The use of this approach was illustrated in the text for two constraints and therefore two undetermined multipliers λ_1 and λ_2 (α and $-\beta$).

The multipliers λ cannot always remain undetermined. One approach is to solve eqn A2.50 instead of incorporating it into the minimization scheme. In Chapter 16 we used the alternative procedure of keeping λ undetermined until a property was calculated for which the value was already known. Thus, we found that $\beta = 1/kT$ by calculating the internal energy of a perfect gas.

A2.9 Differential equations

(a) Ordinary differential equations

An **ordinary differential equation** is a relation between derivatives of a function of one variable and the function itself, as in

$$a\frac{\mathrm{d}^2y}{\mathrm{d}x^2}+b\frac{\mathrm{d}y}{\mathrm{d}x}+cy=0 \qquad \text{(A2.54)}$$

The coefficients a, b, etc. may be functions of x. The **order** of the equation is the order of the highest derivative that occurs in it, so eqn A2.54 is a second-order equation. Only rarely in science is a differential equation of order higher than 2 encountered. A solution of a differential equation is an expression for y as a function of x. The process of solving a differential equation is commonly termed 'integration', and in simple cases simple integration can be employed to find $y(x)$. A **general solution** of a differential equation is the most general solution of the equation and is expressed in terms of a number of constants. 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. A first–order differential equation requires the specification of *one* boundary (or initial) condition; a second–order differential equation requires the specification of *two* such conditions, and so on.

First-order differential equations may often be solved by direct integration. For example, the equation

$$\frac{\mathrm{d}y}{\mathrm{d}x}=axy$$

with a constant may be rearranged into

$$\frac{\mathrm{d}y}{y}=a\mathrm{d}x$$

and then integrated to

$$\ln y=\tfrac{1}{2}ax^2+A$$

where A is a constant. If we know that $y=y_0$ when $x=0$ (for instance), then it follows that $A=\ln y_0$, and hence the particular solution of the equation is

$$\ln y=\tfrac{1}{2}ax^2+\ln y_0$$

This expression rearranges to

$$y=y_0\mathrm{e}^{ax^2/2}$$

First-order equations of a more complex form can often be solved by the appropriate substitution. For example, it is sensible to try the substitution $y=sx$, and to change the variables from x and y to x and s. An alternative useful transformation is to write $x=u+a$ and $y=v+b$, and then to select a and b to simplify the form of the resulting expression.

Solutions to complicated differential equations may also be found by referring to tables (see *Further reading*). For example, first-order equations of the form

$$\frac{\mathrm{d}y}{\mathrm{d}x}+yf(x)=g(x) \qquad \text{(A2.55)}$$

appear in the study of chemical kinetics. The solution is given by

$$ye^{\int f(x)dx} = \int e^{\int f(x)dx} g(x)dx + \text{constant} \tag{A2.56}$$

Mathematical software is now capable of finding analytical solutions of a wide variety of differential equations.

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:

$$y = \sum_{n=0}^{\infty} c_n x^n \tag{A2.57}$$

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 (Section 9.4). All 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.

(b) Numerical integration of differential equations

Many of the differential equations that describe physical phenomena are so complicated that their solutions cannot be cast as functions. In such cases, we resort to numerical methods, in which approximations are made in order to integrate the differential equation. Software packages are now readily available that can be used to solve almost any equation numerically. The general form of such programs to solve $df/dx = g(x)$, for instance, replaces the infinitesimal quantity $df = g(x)dx$ by the small quantity $\Delta f = g(x)\Delta x$, so that

$$f(x + \Delta x) \approx f(x) + g(x)\Delta x$$

and then proceeds numerically to step along the x-axis, generating $f(x)$ as it goes. The actual algorithms adopted are much more sophisticated than this primitive scheme, but stem from it. Among the simple numerical methods, the fourth-order **Runge–Kutta method** is one of the most accurate.

The *Further reading* section lists monographs that discuss the derivation of the fourth-order Runge–Kutta method. Here we illustrate the procedure with a first-order differential equation of the form:

$$\frac{dy}{dx} = f(x,y) \tag{A2.58}$$

One example of this differential equation in chemical kinetics is eqn 22.36, which describes the time dependence of the concentration of an intermediate I in the reaction sequence $A \rightarrow I \rightarrow P$.

To obtain an approximate value of the integral of eqn A2.58, we proceed by rewriting it in terms of finite differences instead of differentials:

$$\frac{\Delta y}{\Delta x} = f(x,y)$$

where Δy may also be written as $y(x + \Delta x) - y(x)$. The fourth-order Runge–Kutta method is based on the following approximation:

$$y(x + \Delta x) = y(x) + \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{A2.59}$$