11.7 Integral forms for grad, div and curl

In the previous chapter we defined the vector operators grad, div and curl in purely mathematical terms, which depended on the coordinate system in which they were expressed. An interesting application of line, surface and volume integrals is the expression of grad, div and curl in coordinate-free, geometrical terms. If ϕ is a scalar field and $\mathbf{a}$ is a vector field then it may be shown that at any point P

$$\nabla\phi = \lim_{V\to 0}\left(\frac{1}{V}\oint_S \phi\, d\mathbf{S}\right) \tag{11.14}$$

$$\nabla\cdot\mathbf{a} = \lim_{V\to 0}\left(\frac{1}{V}\oint_S \mathbf{a}\cdot d\mathbf{S}\right) \tag{11.15}$$

$$\nabla\times\mathbf{a} = \lim_{V\to 0}\left(\frac{1}{V}\oint_S d\mathbf{S}\times\mathbf{a}\right) \tag{11.16}$$

where V is a small volume enclosing P and S is its bounding surface. Indeed, we may consider these equations as the (geometrical) *definitions* of grad, div and curl. An alternative, but equivalent, geometrical definition of $\nabla\times\mathbf{a}$ at a point P, which is often easier to use than (11.16), is given by

$$(\nabla\times\mathbf{a})\cdot\hat{\mathbf{n}} = \lim_{A\to 0}\left(\frac{1}{A}\oint_C \mathbf{a}\cdot d\mathbf{r}\right), \tag{11.17}$$

where C is a plane contour of area A enclosing the point P and $\hat{\mathbf{n}}$ is the unit normal to the enclosed planar area.

It may be shown, *in any coordinate system*, that all the above equations are consistent with our definitions in the previous chapter, although the difficulty of proof depends on the chosen coordinate system. The most general coordinate system encountered in that chapter was one with orthogonal curvilinear coordinates u_1, u_2, u_3, of which Cartesians, cylindrical polars and spherical polars are all special cases. Although it may be shown that (11.14) leads to the usual expression for grad in curvilinear coordinates, the proof requires complicated manipulations of the derivatives of the basis vectors with respect to the coordinates and is not presented here. In Cartesian coordinates, however, the proof is quite simple.

►*Show that the geometrical definition of* grad *leads to the usual expression for* $\nabla\phi$ *in Cartesian coordinates.*

Consider the surface S of a small rectangular volume element $\Delta V = \Delta x\,\Delta y\,\Delta z$ that has its faces parallel to the x, y, and z coordinate surfaces; the point P (see above) is at one corner. We must calculate the surface integral (11.14) over each of its six faces. Remembering that the normal to the surface points outwards from the volume on each face, the two faces with $x =$ constant have areas $\Delta\mathbf{S} = -\mathbf{i}\,\Delta y\,\Delta z$ and $\Delta\mathbf{S} = \mathbf{i}\,\Delta y\,\Delta z$ respectively. Furthermore, over each small surface element, we may take ϕ to be constant, so that the net contribution to the surface integral from these two faces is then

$$\begin{aligned}[(\phi+\Delta\phi)-\phi]\,\Delta y\,\Delta z\,\mathbf{i} &= \left(\phi+\frac{\partial\phi}{\partial x}\Delta x-\phi\right)\,\Delta y\,\Delta z\,\mathbf{i}\\ &= \frac{\partial\phi}{\partial x}\,\Delta x\,\Delta y\,\Delta z\,\mathbf{i}.\end{aligned}$$

The surface integral over the pairs of faces with $y =$ constant and $z =$ constant respectively may be found in a similar way, and we obtain

$$\oint_S \phi\, d\mathbf{S} = \left(\frac{\partial\phi}{\partial x}\mathbf{i}+\frac{\partial\phi}{\partial y}\mathbf{j}+\frac{\partial\phi}{\partial z}\mathbf{k}\right)\,\Delta x\,\Delta y\,\Delta z.$$

Therefore $\nabla\phi$ at the point P is given by

$$\begin{aligned}\nabla\phi &= \lim_{\Delta x,\Delta y,\Delta z\to 0}\left[\frac{1}{\Delta x\,\Delta y\,\Delta z}\left(\frac{\partial\phi}{\partial x}\mathbf{i}+\frac{\partial\phi}{\partial y}\mathbf{j}+\frac{\partial\phi}{\partial z}\mathbf{k}\right)\,\Delta x\,\Delta y\,\Delta z\right]\\ &= \frac{\partial\phi}{\partial x}\mathbf{i}+\frac{\partial\phi}{\partial y}\mathbf{j}+\frac{\partial\phi}{\partial z}\mathbf{k}.\ \blacktriangleleft\end{aligned}$$

We now turn to (11.15) and (11.17). These geometrical definitions may be shown straightforwardly to lead to the usual expressions for div and curl in orthogonal curvilinear coordinates.

►*By considering the infinitesimal volume element $dV = h_1h_2h_3\,\Delta u_1\,\Delta u_2\,\Delta u_3$ shown in figure 11.10, show that (11.15) leads to the usual expression for $\nabla\cdot\mathbf{a}$ in orthogonal curvilinear coordinates.*

Let us write the vector field in terms of its components with respect to the basis vectors of the curvilinear coordinate system as $\mathbf{a} = a_1\hat{\mathbf{e}}_1 + a_2\hat{\mathbf{e}}_2 + a_3\hat{\mathbf{e}}_3$. We consider first the contribution to the RHS of (11.15) from the two faces with $u_1 =$ constant, i.e. $PQRS$ and the face opposite it (see figure 11.10). Now, the volume element is formed from the orthogonal vectors $h_1\,\Delta u_1\,\hat{\mathbf{e}}_1$, $h_2\,\Delta u_2\,\hat{\mathbf{e}}_2$ and $h_3\,\Delta u_3\,\hat{\mathbf{e}}_3$ at the point P and so for $PQRS$ we have

$$\Delta\mathbf{S} = h_2h_3\,\Delta u_2\,\Delta u_3\;\hat{\mathbf{e}}_3\times\hat{\mathbf{e}}_2 = -h_2h_3\,\Delta u_2\,\Delta u_3\,\hat{\mathbf{e}}_1.$$

Reasoning along the same lines as in the previous example, we conclude that the contribution to the surface integral of $\mathbf{a}\cdot d\mathbf{S}$ over $PQRS$ and its opposite face taken together is given by

$$\frac{\partial}{\partial u_1}(\mathbf{a}\cdot\Delta\mathbf{S})\,\Delta u_1 = \frac{\partial}{\partial u_1}(a_1h_2h_3)\,\Delta u_1\,\Delta u_2\,\Delta u_3.$$

The surface integrals over the pairs of faces with $u_2 =$ constant and $u_3 =$ constant respectively may be found in a similar way, and we obtain

$$\oint_S \mathbf{a}\cdot d\mathbf{S} = \left[\frac{\partial}{\partial u_1}(a_1h_2h_3)+\frac{\partial}{\partial u_2}(a_2h_3h_1)+\frac{\partial}{\partial u_3}(a_3h_1h_2)\right]\,\Delta u_1\,\Delta u_2\,\Delta u_3.$$

Therefore $\nabla\cdot\mathbf{a}$ at the point P is given by

$$\begin{aligned}\nabla\cdot\mathbf{a} &= \lim_{\Delta u_1,\Delta u_2,\Delta u_3\to 0}\left[\frac{1}{h_1h_2h_3\,\Delta u_1\,\Delta u_2\,\Delta u_3}\oint_S \mathbf{a}\cdot d\mathbf{S}\right]\\ &= \frac{1}{h_1h_2h_3}\left[\frac{\partial}{\partial u_1}(a_1h_2h_3)+\frac{\partial}{\partial u_2}(a_2h_3h_1)+\frac{\partial}{\partial u_3}(a_3h_1h_2)\right].\ \blacktriangleleft\end{aligned}$$

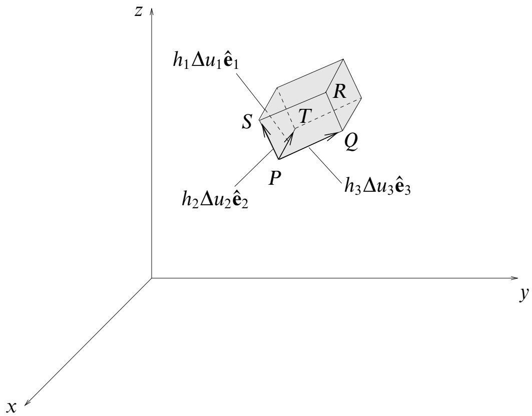

Figure 11.10 A general volume ΔV in orthogonal curvilinear coordinates u_1, u_2, u_3. PT gives the vector $h_1\,\Delta u_1\,\hat{\mathbf{e}}_1$, PS gives $h_2\,\Delta u_2\,\hat{\mathbf{e}}_2$ and PQ gives $h_3\,\Delta u_3\,\hat{\mathbf{e}}_3$.

►*By considering the infinitesimal planar surface element $PQRS$ in figure 11.10, show that (11.17) leads to the usual expression for $\nabla \times \mathbf{a}$ in orthogonal curvilinear coordinates.*

The planar surface $PQRS$ is defined by the orthogonal vectors $h_2\,\Delta u_2\,\hat{\mathbf{e}}_2$ and $h_3\,\Delta u_3\,\hat{\mathbf{e}}_3$ at the point P. If we traverse the loop in the direction $PSRQ$ then, by the right-hand convention, the unit normal to the plane is $\hat{\mathbf{e}}_1$. Writing $\mathbf{a} = a_1\hat{\mathbf{e}}_1 + a_2\hat{\mathbf{e}}_2 + a_3\hat{\mathbf{e}}_3$, the line integral around the loop in this direction is given by

$$\begin{aligned}\oint_{PSRQ} \mathbf{a} \cdot d\mathbf{r} &= a_2 h_2\,\Delta u_2 + \left[a_3 h_3 + \frac{\partial}{\partial u_2}(a_3 h_3)\,\Delta u_2\right]\,\Delta u_3 \\ &\qquad - \left[a_2 h_2 + \frac{\partial}{\partial u_3}(a_2 h_2)\,\Delta u_3\right]\,\Delta u_2 - a_3 h_3\,\Delta u_3 \\ &= \left[\frac{\partial}{\partial u_2}(a_3 h_3) - \frac{\partial}{\partial u_3}(a_2 h_2)\right]\,\Delta u_2\,\Delta u_3.\end{aligned}$$

Therefore from (11.17) the component of $\nabla \times \mathbf{a}$ in the direction $\hat{\mathbf{e}}_1$ at P is given by

$$\begin{aligned}(\nabla \times \mathbf{a})_1 &= \lim_{\Delta u_2, \Delta u_3 \to 0}\left[\frac{1}{h_2 h_3\,\Delta u_2\,\Delta u_3}\oint_{PSRQ} \mathbf{a} \cdot d\mathbf{r}\right] \\ &= \frac{1}{h_2 h_3}\left[\frac{\partial}{\partial u_2}(h_3 a_3) - \frac{\partial}{\partial u_3}(h_2 a_2)\right].\end{aligned}$$

The other two components are found by cyclically permuting the subscripts 1, 2, 3. ◄

Finally, we note that we can also write the ∇^2 operator as a surface integral by setting $\mathbf{a} = \nabla\phi$ in (11.15), to obtain

$$\nabla^2\phi = \nabla \cdot \nabla\phi = \lim_{V \to 0}\left(\frac{1}{V}\oint_S \nabla\phi \cdot d\mathbf{S}\right).$$

11.8 Divergence theorem and related theorems

The divergence theorem relates the total flux of a vector field out of a closed surface S to the integral of the divergence of the vector field over the enclosed volume V; it follows almost immediately from our geometrical definition of divergence (11.15).

Imagine a volume V, in which a vector field $\mathbf{a}$ is continuous and differentiable, to be divided up into a large number of small volumes V_i. Using (11.15), we have for each small volume

$$(\nabla \cdot \mathbf{a})V_i \approx \oint_{S_i} \mathbf{a} \cdot d\mathbf{S},$$

where S_i is the surface of the small volume V_i. Summing over i we find that contributions from surface elements interior to S cancel since each surface element appears in two terms with opposite signs, the outward normals in the two terms being equal and opposite. Only contributions from surface elements that are also parts of S survive. If each V_i is allowed to tend to zero then we obtain the *divergence theorem*,

$$\int_V \nabla \cdot \mathbf{a}\, dV = \oint_S \mathbf{a} \cdot d\mathbf{S}. \tag{11.18}$$

We note that the divergence theorem holds for both simply and multiply connected surfaces, provided that they are closed and enclose some non-zero volume V. The divergence theorem may also be extended to tensor fields (see chapter 26).

The theorem finds most use as a tool in formal manipulations, but sometimes it is of value in transforming surface integrals of the form $\int_S \mathbf{a} \cdot d\mathbf{S}$ into volume integrals or vice versa. For example, setting $\mathbf{a} = \mathbf{r}$ we immediately obtain

$$\int_V \nabla \cdot \mathbf{r}\, dV = \int_V 3\, dV = 3V = \oint_S \mathbf{r} \cdot d\mathbf{S},$$

which gives the expression for the volume of a region found in subsection 11.6.1. The use of the divergence theorem is further illustrated in the following example.

►*Evaluate the surface integral $I = \int_S \mathbf{a} \cdot d\mathbf{S}$, where $\mathbf{a} = (y - x)\,\mathbf{i} + x^2 z\,\mathbf{j} + (z + x^2)\,\mathbf{k}$ and S is the open surface of the hemisphere $x^2 + y^2 + z^2 = a^2$, $z \geq 0$.*

We could evaluate this surface integral directly, but the algebra is somewhat lengthy. We will therefore evaluate it by use of the divergence theorem. Since the latter only holds for closed surfaces enclosing a non-zero volume V, let us first consider the closed surface $S' = S + S_1$, where S_1 is the circular area in the xy-plane given by $x^2 + y^2 \leq a^2$, $z = 0$; S' then encloses a hemispherical volume V. By the divergence theorem we have

$$\int_V \nabla \cdot \mathbf{a}\, dV = \oint_{S'} \mathbf{a} \cdot d\mathbf{S} = \int_S \mathbf{a} \cdot d\mathbf{S} + \int_{S_1} \mathbf{a} \cdot d\mathbf{S}.$$

Now $\nabla \cdot \mathbf{a} = -1 + 0 + 1 = 0$, so we can write

$$\int_S \mathbf{a} \cdot d\mathbf{S} = -\int_{S_1} \mathbf{a} \cdot d\mathbf{S}.$$

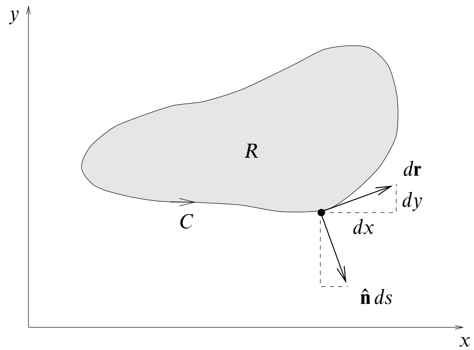

Figure 11.11 A closed curve C in the xy-plane bounding a region R. Vectors tangent and normal to the curve at a given point are also shown.

The surface integral over S_1 is easily evaluated. Remembering that the normal to the surface points outward from the volume, a surface element on S_1 is simply $d\mathbf{S} = -\mathbf{k}\,dx\,dy$. On S_1 we also have $\mathbf{a} = (y - x)\,\mathbf{i} + x^2\,\mathbf{k}$, so that

$$I = -\int_{S_1} \mathbf{a} \cdot d\mathbf{S} = \iint_R x^2\,dx\,dy,$$

where R is the circular region in the xy-plane given by $x^2 + y^2 \leq a^2$. Transforming to plane polar coordinates we have

$$I = \iint_{R'} \rho^2 \cos^2\phi \;\rho\,d\rho\,d\phi = \int_0^{2\pi} \cos^2\phi\,d\phi \int_0^a \rho^3\,d\rho = \frac{\pi a^4}{4}. \blacktriangleleft$$

It is also interesting to consider the two-dimensional version of the divergence theorem. As an example, let us consider a two-dimensional planar region R in the xy-plane bounded by some closed curve C (see figure 11.11). At any point on the curve the vector $d\mathbf{r} = dx\,\mathbf{i} + dy\,\mathbf{j}$ is a tangent to the curve and the vector $\hat{\mathbf{n}}\,ds = dy\,\mathbf{i} - dx\,\mathbf{j}$ is a normal pointing out of the region R. If the vector field $\mathbf{a}$ is continuous and differentiable in R then the two-dimensional divergence theorem in Cartesian coordinates gives

$$\iint_R \left(\frac{\partial a_x}{\partial x} + \frac{\partial a_y}{\partial y} \right) dx\,dy = \oint \mathbf{a} \cdot \hat{\mathbf{n}}\,ds = \oint_C (a_x\,dy - a_y\,dx).$$

Letting $P = -a_y$ and $Q = a_x$, we recover Green's theorem in a plane, which was discussed in section 11.3.

11.8.1 Green's theorems

Consider two scalar functions ϕ and ψ that are continuous and differentiable in some volume V bounded by a surface S. Applying the divergence theorem to the vector field $\phi\nabla\psi$ we obtain

$$\oint_S \phi\nabla\psi \cdot d\mathbf{S} = \int_V \nabla\cdot(\phi\nabla\psi)\,dV$$
$$= \int_V \left[\phi\nabla^2\psi + (\nabla\phi)\cdot(\nabla\psi)\right]\,dV. \qquad (11.19)$$

Reversing the roles of ϕ and ψ in (11.19) and subtracting the two equations gives

$$\oint_S (\phi\nabla\psi - \psi\nabla\phi)\cdot d\mathbf{S} = \int_V (\phi\nabla^2\psi - \psi\nabla^2\phi)\,dV. \qquad (11.20)$$

Equation (11.19) is usually known as Green's first theorem and (11.20) as his second. Green's second theorem is useful in the development of the Green's functions used in the solution of partial differential equations (see chapter 21).

11.8.2 Other related integral theorems

There exist two other integral theorems which are closely related to the divergence theorem and which are of some use in physical applications. If ϕ is a scalar field and $\mathbf{b}$ is a vector field and both ϕ and $\mathbf{b}$ satisfy our usual differentiability conditions in some volume V bounded by a closed surface S then

$$\int_V \nabla\phi\,dV = \oint_S \phi\,d\mathbf{S}, \qquad (11.21)$$

$$\int_V \nabla\times\mathbf{b}\,dV = \oint_S d\mathbf{S}\times\mathbf{b}. \qquad (11.22)$$

►*Use the divergence theorem to prove (11.21).*

In the divergence theorem (11.18) let $\mathbf{a} = \phi\mathbf{c}$, where $\mathbf{c}$ is a constant vector. We then have

$$\int_V \nabla\cdot(\phi\mathbf{c})\,dV = \oint_S \phi\mathbf{c}\cdot d\mathbf{S}.$$

Expanding out the integrand on the LHS we have

$$\nabla\cdot(\phi\mathbf{c}) = \phi\nabla\cdot\mathbf{c} + \mathbf{c}\cdot\nabla\phi = \mathbf{c}\cdot\nabla\phi,$$

since $\mathbf{c}$ is constant. Also, $\phi\mathbf{c}\cdot d\mathbf{S} = \mathbf{c}\cdot\phi d\mathbf{S}$, so we obtain

$$\int_V \mathbf{c}\cdot(\nabla\phi)\,dV = \oint_S \mathbf{c}\cdot\phi\,d\mathbf{S}.$$

Since $\mathbf{c}$ is constant we may take it out of both integrals to give

$$\mathbf{c}\cdot\int_V \nabla\phi\,dV = \mathbf{c}\cdot\oint_S \phi\,d\mathbf{S},$$

and since $\mathbf{c}$ is arbitrary we obtain the stated result (11.21). ◄

Equation (11.22) may be proved in a similar way by letting $\mathbf{a} = \mathbf{b}\times\mathbf{c}$ in the divergence theorem, where $\mathbf{c}$ is again a constant vector.

11.8.3 Physical applications of the divergence theorem

The divergence theorem is useful in deriving many of the most important partial differential equations in physics (see chapter 20). The basic idea is to use the divergence theorem to convert an integral form, often derived from observation, into an equivalent differential form (used in theoretical statements).

►*For a compressible fluid with time-varying position-dependent density $\rho(\mathbf{r}, t)$ and velocity field $v(\mathbf{r}, t)$, in which fluid is neither being created nor destroyed, show that*

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0.$$

For an arbitrary volume V in the fluid, the conservation of mass tells us that the rate of increase or decrease of the mass M of fluid in the volume must equal the net rate at which fluid is entering or leaving the volume, i.e.

$$\frac{dM}{dt} = -\oint_S \rho \mathbf{v} \cdot d\mathbf{S},$$

where S is the surface bounding V. But the mass of fluid in V is simply $M = \int_V \rho\, dV$, so we have

$$\frac{d}{dt}\int_V \rho\, dV + \oint_S \rho \mathbf{v} \cdot d\mathbf{S} = 0.$$

Taking the derivative inside the first integral on the RHS and using the divergence theorem to rewrite the second integral, we obtain

$$\int_V \frac{\partial \rho}{\partial t}\, dV + \int_V \nabla \cdot (\rho \mathbf{v})\, dV = \int_V \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v})\right] dV = 0.$$

Since the volume V is arbitrary, the integrand (which is assumed continuous) must be identically zero, so we obtain

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0.$$

This is known as the *continuity equation*. It can also be applied to other systems, for example those in which ρ is the density of electric charge or the heat content, etc. For the flow of an incompressible fluid, $\rho =$ constant and the continuity equation becomes simply $\nabla \cdot \mathbf{v} = 0$. ◄

In the previous example, we assumed that there were no sources or sinks in the volume V, i.e. that there was no part of V in which fluid was being created or destroyed. We now consider the case where a finite number of *point* sources and/or sinks are present in an incompressible fluid. Let us first consider the simple case where a single source is located at the origin, out of which a quantity of fluid flows radially at a rate Q ($\mathrm{m}^3\ \mathrm{s}^{-1}$). The velocity field is given by

$$\mathbf{v} = \frac{Q\mathbf{r}}{4\pi r^3} = \frac{Q\hat{\mathbf{r}}}{4\pi r^2}.$$

Now, for a sphere S_1 of radius r centred on the source, the flux across S_1 is

$$\oint_{S_1} \mathbf{v} \cdot d\mathbf{S} = |\mathbf{v}| 4\pi r^2 = Q.$$

Since $\mathbf{v}$ has a singularity at the origin it is not differentiable there, i.e. $\nabla \cdot \mathbf{v}$ is not defined there, but at all other points $\nabla \cdot \mathbf{v} = 0$, as required for an incompressible fluid. Therefore, from the divergence theorem, for any closed surface S_2 that does not enclose the origin we have

$$\oint_{S_2} \mathbf{v} \cdot d\mathbf{S} = \int_V \nabla \cdot \mathbf{v}\, dV = 0.$$

Thus we see that the surface integral $\oint_S \mathbf{v} \cdot d\mathbf{S}$ has value Q or zero depending on whether or not S encloses the source. In order that the divergence theorem is valid for *all* surfaces S, irrespective of whether they enclose the source, we write

$$\nabla \cdot \mathbf{v} = Q\delta(\mathbf{r}),$$

where $\delta(\mathbf{r})$ is the three-dimensional Dirac delta function. The properties of this function are discussed fully in chapter 13, but for the moment we note that it is defined in such a way that

$$\delta(\mathbf{r} - \mathbf{a}) = 0 \qquad \text{for } \mathbf{r} \neq \mathbf{a},$$

$$\int_V f(\mathbf{r})\delta(\mathbf{r} - \mathbf{a})\, dV = \begin{cases} f(\mathbf{a}) & \text{if } \mathbf{a} \text{ lies in } V \\ 0 & \text{otherwise} \end{cases}$$

for any well-behaved function $f(\mathbf{r})$. Therefore, for any volume V containing the source at the origin, we have

$$\int_V \nabla \cdot \mathbf{v}\, dV = Q \int_V \delta(\mathbf{r})\, dV = Q,$$

which is consistent with $\oint_S \mathbf{v} \cdot d\mathbf{S} = Q$ for a closed surface enclosing the source. Hence, by introducing the Dirac delta function the divergence theorem can be made valid even for non-differentiable point sources.

The generalisation to several sources and sinks is straightforward. For example, if a source is located at $\mathbf{r} = \mathbf{a}$ and a sink at $\mathbf{r} = \mathbf{b}$ then the velocity field is

$$\mathbf{v} = \frac{(\mathbf{r} - \mathbf{a})Q}{4\pi|\mathbf{r} - \mathbf{a}|^3} - \frac{(\mathbf{r} - \mathbf{b})Q}{4\pi|\mathbf{r} - \mathbf{b}|^3}$$

and its divergence is given by

$$\nabla \cdot \mathbf{v} = Q\delta(\mathbf{r} - \mathbf{a}) - Q\delta(\mathbf{r} - \mathbf{b}).$$

Therefore, the integral $\oint_S \mathbf{v} \cdot d\mathbf{S}$ has the value Q if S encloses the source, $-Q$ if S encloses the sink and 0 if S encloses neither the source nor sink or encloses them both. This analysis also applies to other physical systems – for example, in electrostatics we can regard the sources and sinks as positive and negative point charges respectively and replace $\mathbf{v}$ by the electric field $\mathbf{E}$.

11.9 Stokes' theorem and related theorems

Stokes' theorem is the 'curl analogue' of the divergence theorem and relates the integral of the curl of a vector field over an open surface S to the line integral of the vector field around the perimeter C bounding the surface.

Following the same lines as for the derivation of the divergence theorem, we can divide the surface S into many small areas S_i with boundaries C_i and unit normals $\hat{\mathbf{n}}_i$. Using (11.17), we have for each small area

$$(\nabla \times \mathbf{a}) \cdot \hat{\mathbf{n}}_i \; S_i \approx \oint_{C_i} \mathbf{a} \cdot d\mathbf{r}.$$

Summing over i we find that on the RHS all parts of all interior boundaries that are not part of C are included twice, being traversed in opposite directions on each occasion and thus contributing nothing. Only contributions from line elements that are also parts of C survive. If each S_i is allowed to tend to zero then we obtain Stokes' theorem,

$$\int_S (\nabla \times \mathbf{a}) \cdot d\mathbf{S} = \oint_C \mathbf{a} \cdot d\mathbf{r}. \tag{11.23}$$

We note that Stokes' theorem holds for both simply and multiply connected open surfaces, provided that they are two-sided. Stokes' theorem may also be extended to tensor fields (see chapter 26).

Just as the divergence theorem (11.18) can be used to relate volume and surface integrals for certain types of integrand, Stokes' theorem can be used in evaluating surface integrals of the form $\oint_S (\nabla \times \mathbf{a}) \cdot d\mathbf{S}$ as line integrals or vice versa.

►*Given the vector field* $\mathbf{a} = y\,\mathbf{i} - x\,\mathbf{j} + z\,\mathbf{k}$, *verify Stokes' theorem for the hemispherical surface* $x^2 + y^2 + z^2 = a^2$, $z \geq 0$.

Let us first evaluate the surface integral

$$\int_S (\nabla \times \mathbf{a}) \cdot d\mathbf{S}$$

over the hemisphere. It is easily shown that $\nabla \times \mathbf{a} = -2\,\mathbf{k}$, and the surface element is $d\mathbf{S} = a^2 \sin\theta \, d\theta \, d\phi \; \hat{\mathbf{r}}$ in spherical polar coordinates. Therefore

$$\begin{aligned} \int_S (\nabla \times \mathbf{a}) \cdot d\mathbf{S} &= \int_0^{2\pi} d\phi \int_0^{\pi/2} d\theta \, \left(-2a^2 \sin\theta\right) \hat{\mathbf{r}} \cdot \mathbf{k} \\ &= -2a^2 \int_0^{2\pi} d\phi \int_0^{\pi/2} \sin\theta \left(\frac{z}{a}\right) \, d\theta \\ &= -2a^2 \int_0^{2\pi} d\phi \int_0^{\pi/2} \sin\theta \cos\theta \, d\theta = -2\pi a^2. \end{aligned}$$

We now evaluate the line integral around the perimeter curve C of the surface, which is the circle $x^2 + y^2 = a^2$ in the xy-plane. This is given by

$$\oint_C \mathbf{a} \cdot d\mathbf{r} = \oint_C (y\,\mathbf{i} - x\,\mathbf{j} + z\,\mathbf{k}) \cdot (dx\,\mathbf{i} + dy\,\mathbf{j} + dz\,\mathbf{k})$$
$$= \oint_C (y\,dx - x\,dy).$$

Using plane polar coordinates, on C we have $x = a\cos\phi$, $y = a\sin\phi$ so that $dx = -a\sin\phi\,d\phi$, $dy = a\cos\phi\,d\phi$, and the line integral becomes

$$\oint_C (y\,dx - x\,dy) = -a^2 \int_0^{2\pi} (\sin^2\phi + \cos^2\phi)\,d\phi = -a^2 \int_0^{2\pi} d\phi = -2\pi a^2.$$

Since the surface and line integrals have the same value, we have verified Stokes' theorem in this case. ◄

The two-dimensional version of Stokes' theorem also yields Green's theorem in a plane. Consider the region R in the xy-plane shown in figure 11.11, in which a vector field $\mathbf{a}$ is defined. Since $\mathbf{a} = a_x\,\mathbf{i} + a_y\,\mathbf{j}$, we have $\nabla \times \mathbf{a} = (\partial a_y/\partial x - \partial a_x/\partial y)\,\mathbf{k}$, and Stokes' theorem becomes

$$\iint_R \left(\frac{\partial a_y}{\partial x} - \frac{\partial a_x}{\partial y} \right) dx\,dy = \oint_C (a_x\,dx + a_y\,dy).$$

Letting $P = a_x$ and $Q = a_y$ we recover Green's theorem in a plane, (11.4).

11.9.1 Related integral theorems

As for the divergence theorem, there exist two other integral theorems that are closely related to Stokes' theorem. If ϕ is a scalar field and $\mathbf{b}$ is a vector field, and both ϕ and $\mathbf{b}$ satisfy our usual differentiability conditions on some two-sided open surface S bounded by a closed perimeter curve C, then

$$\int_S d\mathbf{S} \times \nabla\phi = \oint_C \phi\,d\mathbf{r}, \tag{11.24}$$

$$\int_S (d\mathbf{S} \times \nabla) \times \mathbf{b} = \oint_C d\mathbf{r} \times \mathbf{b}. \tag{11.25}$$

►*Use Stokes' theorem to prove (11.24).*

In Stokes' theorem, (11.23), let $\mathbf{a} = \phi\mathbf{c}$, where $\mathbf{c}$ is a constant vector. We then have

$$\int_S [\nabla \times (\phi\mathbf{c})] \cdot d\mathbf{S} = \oint_C \phi\mathbf{c} \cdot d\mathbf{r}. \tag{11.26}$$

Expanding out the integrand on the LHS we have

$$\nabla \times (\phi\mathbf{c}) = \nabla\phi \times \mathbf{c} + \phi\nabla \times \mathbf{c} = \nabla\phi \times \mathbf{c},$$

since $\mathbf{c}$ is constant, and the scalar triple product on the LHS of (11.26) can therefore be written

$$[\nabla \times (\phi\mathbf{c})] \cdot d\mathbf{S} = (\nabla\phi \times \mathbf{c}) \cdot d\mathbf{S} = \mathbf{c} \cdot (d\mathbf{S} \times \nabla\phi).$$

Substituting this into (11.26) and taking $\mathbf{c}$ out of both integrals because it is constant, we find

$$\mathbf{c} \cdot \int_S d\mathbf{S} \times \nabla\phi = \mathbf{c} \cdot \oint_C \phi\, d\mathbf{r}.$$

Since $\mathbf{c}$ is an arbitrary constant vector we therefore obtain the stated result (11.24). ◄

Equation (11.25) may be proved in a similar way, by letting $\mathbf{a} = \mathbf{b} \times \mathbf{c}$ in Stokes' theorem, where $\mathbf{c}$ is again a constant vector. We also note that by setting $\mathbf{b} = \mathbf{r}$ in (11.25) we find

$$\int_S (d\mathbf{S} \times \nabla) \times \mathbf{r} = \oint_C d\mathbf{r} \times \mathbf{r}.$$

Expanding out the integrand on the LHS gives

$$(d\mathbf{S} \times \nabla) \times \mathbf{r} = d\mathbf{S} - d\mathbf{S}(\nabla \cdot \mathbf{r}) = d\mathbf{S} - 3\, d\mathbf{S} = -2\, d\mathbf{S}.$$

Therefore, as we found in subsection 11.5.2, the vector area of an open surface S is given by

$$\mathbf{S} = \int_S d\mathbf{S} = \frac{1}{2} \oint_C \mathbf{r} \times d\mathbf{r}.$$

11.9.2 Physical applications of Stokes' theorem

Like the divergence theorem, Stokes' theorem is useful in converting integral equations into differential equations.

►*From Ampère's law, derive Maxwell's equation in the case where the currents are steady, i.e.* $\nabla \times \mathbf{B} - \mu_0 \mathbf{J} = \mathbf{0}$.

Ampère's rule for a distributed current with current density $\mathbf{J}$ is

$$\oint_C \mathbf{B} \cdot d\mathbf{r} = \mu_0 \int_S \mathbf{J} \cdot d\mathbf{S},$$

for any circuit C bounding a surface S. Using Stokes' theorem, the LHS can be transformed into $\int_S (\nabla \times \mathbf{B}) \cdot d\mathbf{S}$; hence

$$\int_S (\nabla \times \mathbf{B} - \mu_0 \mathbf{J}) \cdot d\mathbf{S} = 0$$

for *any* surface S. This can only be so if $\nabla \times \mathbf{B} - \mu_0 \mathbf{J} = \mathbf{0}$, which is the required relation. Similarly, from Faraday's law of electromagnetic induction we can derive Maxwell's equation $\nabla \times \mathbf{E} = -\partial \mathbf{B}/\partial t$. ◄

In subsection 11.8.3 we discussed the flow of an incompressible fluid in the presence of several sources and sinks. Let us now consider *vortex* flow in an incompressible fluid with a velocity field

$$\mathbf{v} = \frac{1}{\rho} \hat{\mathbf{e}}_\phi,$$

in cylindrical polar coordinates ρ, ϕ, z. For this velocity field $\nabla \times \mathbf{v}$ equals zero everywhere except on the axis $\rho = 0$, where $\mathbf{v}$ has a singularity. Therefore $\oint_C \mathbf{v} \cdot d\mathbf{r}$ equals zero for any path C that does not enclose the vortex line on the axis and 2π if C does enclose the axis. In order for Stokes' theorem to be valid for all paths C, we therefore set

$$\nabla \times \mathbf{v} = 2\pi\delta(\rho),$$

where $\delta(\rho)$ is the Dirac delta function, to be discussed in subsection 13.1.3. Now, since $\nabla \times \mathbf{v} = \mathbf{0}$, except on the axis $\rho = 0$, there exists a scalar potential ψ such that $\mathbf{v} = \nabla\psi$. It may easily be shown that $\psi = \phi$, the polar angle. Therefore, if C does not enclose the axis then

$$\oint_C \mathbf{v} \cdot d\mathbf{r} = \oint d\phi = 0,$$

and if C does enclose the axis,

$$\oint_C \mathbf{v} \cdot d\mathbf{r} = \Delta\phi = 2\pi n,$$

where n is the number of times we traverse C. Thus ϕ is a multivalued potential.

Similar analyses are valid for other physical systems – for example, in magnetostatics we may replace the vortex lines by current-carrying wires and the velocity field $\mathbf{v}$ by the magnetic field $\mathbf{B}$.

11.10 Exercises

11.1 The vector field $\mathbf{F}$ is defined by

$$\mathbf{F} = 2xz\mathbf{i} + 2yz^2\mathbf{j} + (x^2 + 2y^2z - 1)\mathbf{k}.$$

Calculate $\nabla \times \mathbf{F}$ and deduce that $\mathbf{F}$ can be written $F = \nabla\phi$. Determine the form of ϕ.

11.2 The vector field $\mathbf{Q}$ is defined by

$$\mathbf{Q} = \left[3x^2(y+z) + y^3 + z^3\right]\mathbf{i} + \left[3y^2(z+x) + z^3 + x^3\right]\mathbf{j} + \left[3z^2(x+y) + x^3 + y^3\right]\mathbf{k}.$$

Show that $\mathbf{Q}$ is a conservative field, construct its potential function and hence evaluate the integral $J = \int \mathbf{Q} \cdot d\mathbf{r}$ along any line connecting the point A at $(1, -1, 1)$ to B at $(2, 1, 2)$.

11.3 $\mathbf{F}$ is a vector field $xy^2\mathbf{i} + 2\mathbf{j} + x\mathbf{k}$, and L is a path parameterised by $x = ct$, $y = c/t$, $z = d$ for the range $1 \le t \le 2$. Evaluate (a) $\int_L \mathbf{F}\,dt$, (b) $\int_L \mathbf{F}\,dy$ and (c) $\int_L \mathbf{F} \cdot d\mathbf{r}$.

11.4 By making an appropriate choice for the functions $P(x, y)$ and $Q(x, y)$ that appear in Green's theorem in a plane, show that the integral of $x - y$ over the upper half of the unit circle centred on the origin has the value $-\frac{2}{3}$. Show the same result by direct integration in Cartesian coordinates.

11.5 Determine the point of intersection P, in the first quadrant, of the two ellipses

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \quad \text{and} \quad \frac{x^2}{b^2} + \frac{y^2}{a^2} = 1.$$

Taking $b < a$, consider the contour L that bounds the area in the first quadrant that is common to the two ellipses. Show that the parts of L that lie along the coordinate axes contribute nothing to the line integral around L of $x\,dy - y\,dx$. Using a parameterisation of each ellipse similar to that employed in the example in section 11.3, evaluate the two remaining line integrals and hence find the total area common to the two ellipses.

11.6 By using parameterisations of the form $x = a\cos^n\theta$ and $y = a\sin^n\theta$ for suitable values of n, find the area bounded by the curves

$$x^{2/5} + y^{2/5} = a^{2/5} \quad \text{and} \quad x^{2/3} + y^{2/3} = a^{2/3}.$$

11.7 Evaluate the line integral

$$I = \oint_C \left[y(4x^2 + y^2)\,dx + x(2x^2 + 3y^2)\,dy \right]$$

around the ellipse $x^2/a^2 + y^2/b^2 = 1$.

11.8 Criticise the following 'proof' that $\pi = 0$.

(a) Apply Green's theorem in a plane to the functions $P(x, y) = \tan^{-1}(y/x)$ and $Q(x, y) = \tan^{-1}(x/y)$, taking the region R to be the unit circle centred on the origin.

(b) The RHS of the equality so produced is

$$\int\int_R \frac{y - x}{x^2 + y^2}\,dx\,dy,$$

which, either from symmetry considerations or by changing to plane polar coordinates, can be shown to have zero value.

(c) In the LHS of the equality, set $x = \cos\theta$ and $y = \sin\theta$, yielding $P(\theta) = \theta$ and $Q(\theta) = \pi/2 - \theta$. The line integral becomes

$$\int_0^{2\pi} \left[\left(\frac{\pi}{2} - \theta \right) \cos\theta - \theta \sin\theta \right] d\theta,$$

which has the value 2π.

(d) Thus $2\pi = 0$ and the stated result follows.

11.9 A single-turn coil C of arbitrary shape is placed in a magnetic field $\mathbf{B}$ and carries a current I. Show that the couple acting upon the coil can be written as

$$\mathbf{M} = I \int_C (\mathbf{B} \cdot \mathbf{r})\,d\mathbf{r} - I \int_C \mathbf{B}(\mathbf{r} \cdot d\mathbf{r}).$$

For a planar rectangular coil of sides $2a$ and $2b$ placed with its plane vertical and at an angle ϕ to a uniform horizontal field $\mathbf{B}$, show that $\mathbf{M}$ is, as expected, $4abBI\cos\phi\,\mathbf{k}$.

11.10 Find the vector area $\mathbf{S}$ of the part of the curved surface of the hyperboloid of revolution

$$\frac{x^2}{a^2} - \frac{y^2 + z^2}{b^2} = 1$$

that lies in the region $z \geq 0$ and $a \leq x \leq \lambda a$.

11.11 An axially symmetric solid body with its axis AB vertical is immersed in an incompressible fluid of density ρ_0. Use the following method to show that, whatever the shape of the body, for $\rho = \rho(z)$ in cylindrical polars the Archimedean upthrust is, as expected, $\rho_0 g V$, where V is the volume of the body.

Express the vertical component of the resultant force on the body, $-\int p\,d\mathbf{S}$, where p is the pressure, in terms of an integral; note that $p = -\rho_0 g z$ and that for an annular surface element of width dl, $\mathbf{n} \cdot \mathbf{n}_z\,dl = -d\rho$. Integrate by parts and use the fact that $\rho(z_A) = \rho(z_B) = 0$.

11.12 Show that the expression below is equal to the solid angle subtended by a rectangular aperture, of sides $2a$ and $2b$, at a point on the normal through its centre, and at a distance c from the aperture:

$$\Omega = 4\int_0^b \frac{ac}{(y^2+c^2)(y^2+c^2+a^2)^{1/2}}\,dy.$$

By setting $y = (a^2+c^2)^{1/2}\tan\phi$, change this integral into the form

$$\int_0^{\phi_1} \frac{4ac\cos\phi}{c^2+a^2\sin^2\phi}\,d\phi,$$

where $\tan\phi_1 = b/(a^2+c^2)^{1/2}$, and hence show that

$$\Omega = 4\tan^{-1}\left[\frac{ab}{c(a^2+b^2+c^2)^{1/2}}\right].$$

11.13 A vector field $\mathbf{a}$ is given by $-zxr^{-3}\mathbf{i}-zyr^{-3}\mathbf{j}+(x^2+y^2)r^{-3}\mathbf{k}$, where $r^2 = x^2+y^2+z^2$. Establish that the field is conservative (a) by showing that $\nabla\times\mathbf{a} = \mathbf{0}$, and (b) by constructing its potential function ϕ.

11.14 A vector field $\mathbf{a}$ is given by $(z^2+2xy)\,\mathbf{i}+(x^2+2yz)\,\mathbf{j}+(y^2+2zx)\,\mathbf{k}$. Show that $\mathbf{a}$ is conservative and that the line integral $\int \mathbf{a}\cdot d\mathbf{r}$ along any line joining $(1,1,1)$ and $(1,2,2)$ has the value 11.

11.15 A force $\mathbf{F}(\mathbf{r})$ acts on a particle at $\mathbf{r}$. In which of the following cases can $\mathbf{F}$ be represented in terms of a potential? Where it can, find the potential.

(a) $\mathbf{F} = F_0\left[\mathbf{i}-\mathbf{j}-\dfrac{2(x-y)}{a^2}\mathbf{r}\right]\exp\left(-\dfrac{r^2}{a^2}\right)$;

(b) $\mathbf{F} = \dfrac{F_0}{a}\left[z\mathbf{k}+\dfrac{(x^2+y^2-a^2)}{a^2}\mathbf{r}\right]\exp\left(-\dfrac{r^2}{a^2}\right)$;

(c) $\mathbf{F} = F_0\left[\mathbf{k}+\dfrac{a(\mathbf{r}\times\mathbf{k})}{r^2}\right]$.

11.16 One of Maxwell's electromagnetic equations states that all magnetic fields $\mathbf{B}$ are solenoidal (i.e. $\nabla\cdot\mathbf{B} = 0$). Determine whether each of the following vectors could represent a real magnetic field; where it could, try to find a suitable vector potential $\mathbf{A}$, i.e. such that $\mathbf{B} = \nabla\times\mathbf{A}$. (Hint: seek a vector potential that is parallel to $\nabla\times\mathbf{B}$.):

(a) $\dfrac{B_0 b}{r^3}[(x-y)z\,\mathbf{i}+(x-y)z\,\mathbf{j}+(x^2-y^2)\,\mathbf{k}]$ in Cartesians with $r^2 = x^2+y^2+z^2$;

(b) $\dfrac{B_0 b^3}{r^3}[\cos\theta\ \cos\phi\,\hat{\mathbf{e}}_r - \sin\theta\ \cos\phi\,\hat{\mathbf{e}}_\theta + \sin 2\theta\ \sin\phi\,\hat{\mathbf{e}}_\phi]$ in spherical polars;

(c) $B_0 b^2\left[\dfrac{z\rho}{(b^2+z^2)^2}\,\hat{\mathbf{e}}_\rho + \dfrac{1}{b^2+z^2}\,\hat{\mathbf{e}}_z\right]$ in cylindrical polars.

11.17 The vector field $\mathbf{f}$ has components $y\mathbf{i}-x\mathbf{j}+\mathbf{k}$ and γ is a curve given parametrically by

$$\mathbf{r} = (a-c+c\cos\theta)\mathbf{i}+(b+c\sin\theta)\mathbf{j}+c^2\theta\mathbf{k},\quad 0\le\theta\le 2\pi.$$

Describe the shape of the path γ and show that the line integral $\int_\gamma \mathbf{f}\cdot d\mathbf{r}$ vanishes. Does this result imply that $\mathbf{f}$ is a conservative field?

11.18 A vector field $\mathbf{a} = f(r)\mathbf{r}$ is spherically symmetric and everywhere directed away from the origin. Show that $\mathbf{a}$ is irrotational, but that it is also solenoidal only if $f(r)$ is of the form Ar^{-3}.

11.19 Evaluate the surface integral $\int \mathbf{r} \cdot d\mathbf{S}$, where $\mathbf{r}$ is the position vector, over that part of the surface $z = a^2 - x^2 - y^2$ for which $z \geq 0$, by each of the following methods.

(a) Parameterise the surface as $x = a \sin\theta \cos\phi$, $y = a \sin\theta \sin\phi$, $z = a^2 \cos^2\theta$, and show that

$$\mathbf{r} \cdot d\mathbf{S} = a^4(2\sin^3\theta\cos\theta + \cos^3\theta\sin\theta)\, d\theta\, d\phi.$$

(b) Apply the divergence theorem to the volume bounded by the surface and the plane $z = 0$.

11.20 Obtain an expression for the value ϕ_P at a point P of a scalar function ϕ that satisfies $\nabla^2\phi = 0$, in terms of its value and normal derivative on a surface S that encloses it, by proceeding as follows.

(a) In Green's second theorem, take ψ at any particular point Q as $1/r$, where r is the distance of Q from P. Show that $\nabla^2\psi = 0$, except at $r = 0$.
(b) Apply the result to the doubly connected region bounded by S and a small sphere Σ of radius δ centred on P.
(c) Apply the divergence theorem to show that the surface integral over Σ involving $1/\delta$ vanishes, and prove that the term involving $1/\delta^2$ has the value $4\pi\phi_P$.
(d) Conclude that

$$\phi_P = -\frac{1}{4\pi}\int_S \phi \frac{\partial}{\partial n}\left(\frac{1}{r}\right) dS + \frac{1}{4\pi}\int_S \frac{1}{r}\frac{\partial\phi}{\partial n}\, dS.$$

This important result shows that the value at a point P of a function ϕ that satisfies $\nabla^2\phi = 0$ everywhere within a closed surface S that encloses P may be expressed *entirely* in terms of its value and normal derivative on S. This matter is taken up more generally in connection with Green's functions in chapter 21 and in connection with functions of a complex variable in section 24.10.

11.21 Use result (11.21), together with an appropriately chosen scalar function ϕ, to prove that the position vector $\bar{\mathbf{r}}$ of the centre of mass of an arbitrarily shaped body of volume V and uniform density can be written

$$\bar{\mathbf{r}} = \frac{1}{V}\oint_S \tfrac{1}{2}r^2\, d\mathbf{S}.$$

11.22 A rigid body of volume V and surface S rotates with angular velocity $\boldsymbol{\omega}$. Show that

$$\boldsymbol{\omega} = -\frac{1}{2V}\oint_S \mathbf{u} \times d\mathbf{S},$$

where $\mathbf{u}(\mathbf{x})$ is the velocity of the point $\mathbf{x}$ on the surface S.

11.23 Demonstrate the validity of the divergence theorem:

(a) by calculating the flux of the vector

$$\mathbf{F} = \frac{\alpha\mathbf{r}}{(r^2 + a^2)^{3/2}}$$

through the spherical surface $|\mathbf{r}| = \sqrt{3}a$;
(b) by showing that

$$\nabla \cdot \mathbf{F} = \frac{3\alpha a^2}{(r^2 + a^2)^{5/2}}$$

and evaluating the volume integral of $\nabla \cdot \mathbf{F}$ over the interior of the sphere $|\mathbf{r}| = \sqrt{3}a$. The substitution $r = a\tan\theta$ will prove useful in carrying out the integration.

11.24 Prove equation (11.22) and, by taking $\mathbf{b} = zx^2\mathbf{i} + zy^2\mathbf{j} + (x^2 - y^2)\mathbf{k}$, show that the two integrals

$$I = \int x^2\,dV \quad \text{and} \quad J = \int \cos^2\theta \sin^3\theta \cos^2\phi\,d\theta\,d\phi,$$

both taken over the unit sphere, must have the same value. Evaluate both directly to show that the common value is $4\pi/15$.

11.25 In a uniform conducting medium with unit relative permittivity, charge density ρ, current density $\mathbf{J}$, electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$, Maxwell's electromagnetic equations take the form (with $\mu_0\epsilon_0 = c^{-2}$)

$$\begin{array}{ll} \text{(i) } \nabla \cdot \mathbf{B} = 0, & \text{(ii) } \nabla \cdot \mathbf{E} = \rho/\epsilon_0, \\ \text{(iii) } \nabla \times \mathbf{E} + \dot{\mathbf{B}} = \mathbf{0}, & \text{(iv) } \nabla \times \mathbf{B} - (\dot{\mathbf{E}}/c^2) = \mu_0\mathbf{J}. \end{array}$$

The density of stored energy in the medium is given by $\frac{1}{2}(\epsilon_0 E^2 + \mu_0^{-1}B^2)$. Show that the rate of change of the total stored energy in a volume V is equal to

$$-\int_V \mathbf{J}\cdot\mathbf{E}\,dV - \frac{1}{\mu_0}\oint_S (\mathbf{E}\times\mathbf{B})\cdot\,d\mathbf{S},$$

where S is the surface bounding V.

[The first integral gives the ohmic heating loss, whilst the second gives the electromagnetic energy flux out of the bounding surface. The vector $\mu_0^{-1}(\mathbf{E}\times\mathbf{B})$ is known as the Poynting vector.]

11.26 A vector field $\mathbf{F}$ is defined in cylindrical polar coordinates ρ, θ, z by

$$\mathbf{F} = F_0\left(\frac{x\cos\lambda z}{a}\mathbf{i} + \frac{y\cos\lambda z}{a}\mathbf{j} + (\sin\lambda z)\mathbf{k}\right) \equiv \frac{F_0\rho}{a}(\cos\lambda z)\mathbf{e}_\rho + F_0(\sin\lambda z)\mathbf{k},$$

where $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ are the unit vectors along the Cartesian axes and $\mathbf{e}_\rho$ is the unit vector $(x/\rho)\mathbf{i} + (y/\rho)\mathbf{j}$.

(a) Calculate, as a surface integral, the flux of $\mathbf{F}$ through the closed surface bounded by the cylinders $\rho = a$ and $\rho = 2a$ and the planes $z = \pm a\pi/2$.
(b) Evaluate the same integral using the divergence theorem.

11.27 The vector field $\mathbf{F}$ is given by

$$\mathbf{F} = (3x^2yz + y^3z + xe^{-x})\mathbf{i} + (3xy^2z + x^3z + ye^x)\mathbf{j} + (x^3y + y^3x + xy^2z^2)\mathbf{k}.$$

Calculate (a) directly, and (b) by using Stokes' theorem the value of the line integral $\int_L \mathbf{F}\cdot d\mathbf{r}$, where L is the (three-dimensional) closed contour $OABCDEO$ defined by the successive vertices $(0,0,0)$, $(1,0,0)$, $(1,0,1)$, $(1,1,1)$, $(1,1,0)$, $(0,1,0)$, $(0,0,0)$.

11.28 A vector force field $\mathbf{F}$ is defined in Cartesian coordinates by

$$\mathbf{F} = F_0\left[\left(\frac{y^3}{3a^3} + \frac{y}{a}e^{xy/a^2} + 1\right)\mathbf{i} + \left(\frac{xy^2}{a^3} + \frac{x+y}{a}e^{xy/a^2}\right)\mathbf{j} + \frac{z}{a}e^{xy/a^2}\mathbf{k}\right].$$

Use Stokes' theorem to calculate

$$\oint_L \mathbf{F}\cdot d\mathbf{r},$$

where L is the perimeter of the rectangle $ABCD$ given by $A = (0,1,0)$, $B = (1,1,0)$, $C = (1,3,0)$ and $D = (0,3,0)$.

11.11 Hints and answers

11.1 Show that $\nabla \times \mathbf{F} = \mathbf{0}$. The potential $\phi_F(\mathbf{r}) = x^2z + y^2z^2 - z$.

11.3 (a) $c^3 \ln 2\,\mathbf{i} + 2\,\mathbf{j} + (3c/2)\mathbf{k}$; (b) $(-3c^4/8)\mathbf{i} - c\,\mathbf{j} - (c^2 \ln 2)\mathbf{k}$; (c) $c^4 \ln 2 - c$.

11.5 For P, $x = y = ab/(a^2 + b^2)^{1/2}$. The relevant limits are $0 \le \theta_1 \le \tan^{-1}(b/a)$ and $\tan^{-1}(a/b) \le \theta_2 \le \pi/2$. The total common area is $4ab\tan^{-1}(b/a)$.

11.7 Show that, in the notation of section 11.3, $\partial Q/\partial x - \partial P/\partial y = 2x^2$; $I = \pi a^3 b/2$.

11.9 $\mathbf{M} = I \int_C \mathbf{r} \times (d\mathbf{r} \times \mathbf{B})$. Show that the horizontal sides in the first term and the whole of the second term contribute nothing to the couple.

11.11 Note that, if $\hat{\mathbf{n}}$ is the outward normal to the surface, $\hat{\mathbf{n}}_z \cdot \hat{\mathbf{n}}\,dl$ is equal to $-d\rho$.

11.13 (b) $\phi = c + z/r$.

11.15 (a) Yes, $F_0(x - y)\exp(-r^2/a^2)$; (b) yes, $-F_0[(x^2 + y^2)/(2a)]\exp(-r^2/a^2)$; (c) no, $\nabla \times \mathbf{F} \neq \mathbf{0}$.

11.17 A spiral of radius c with its axis parallel to the z-direction and passing through (a, b). The pitch of the spiral is $2\pi c^2$. No, because (i) γ is not a closed loop and (ii) the line integral must be zero for *every* closed loop, not just for a particular one. In fact $\nabla \times \mathbf{f} = -2\mathbf{k} \neq \mathbf{0}$ shows that $\mathbf{f}$ is not conservative.

11.19 (a) $d\mathbf{S} = (2a^3 \cos\theta \sin^2\theta \cos\phi\,\mathbf{i} + 2a^3 \cos\theta \sin^2\theta \sin\phi\,\mathbf{j} + a^2 \cos\theta \sin\theta\,\mathbf{k})\,d\theta\,d\phi$.
(b) $\nabla \cdot \mathbf{r} = 3$; over the plane $z = 0$, $\mathbf{r} \cdot d\mathbf{S} = 0$.
The necessarily common value is $3\pi a^4/2$.

11.21 Write $\mathbf{r}$ as $\nabla(\frac{1}{2}r^2)$.

11.23 The answer is $3\sqrt{3}\pi\alpha/2$ in each case.

11.25 Identify the expression for $\nabla \cdot (\mathbf{E} \times \mathbf{B})$ and use the divergence theorem.

11.27 (a) The successive contributions to the integral are:
$1 - 2e^{-1}$, 0, $2 + \frac{1}{2}e$, $-\frac{7}{3}$, $-1 + 2e^{-1}$, $-\frac{1}{2}$.
(b) $\nabla \times \mathbf{F} = 2xyz^2\mathbf{i} - y^2z^2\mathbf{j} + ye^x\mathbf{k}$. Show that the contour is equivalent to the sum of two plane square contours in the planes $z = 0$ and $x = 1$, the latter being traversed in the negative sense. Integral $= \frac{1}{6}(3e - 5)$.

12

Fourier series

We have already discussed, in chapter 4, how complicated functions may be expressed as power series. However, this is not the only way in which a function may be represented as a series, and the subject of this chapter is the expression of functions as a sum of sine and cosine terms. Such a representation is called a *Fourier series*. Unlike Taylor series, a Fourier series can describe functions that are not everywhere continuous and/or differentiable. There are also other advantages in using trigonometric terms. They are easy to differentiate and integrate, their moduli are easily taken and each term contains only one characteristic frequency. This last point is important because, as we shall see later, Fourier series are often used to represent the response of a system to a periodic input, and this response often depends directly on the frequency content of the input. Fourier series are used in a wide variety of such physical situations, including the vibrations of a finite string, the scattering of light by a diffraction grating and the transmission of an input signal by an electronic circuit.

12.1 The Dirichlet conditions

We have already mentioned that Fourier series may be used to represent some functions for which a Taylor series expansion is not possible. The particular conditions that a function $f(x)$ must fulfil in order that it may be expanded as a Fourier series are known as the *Dirichlet conditions*, and may be summarised by the following four points:

(i) the function must be periodic;
(ii) it must be single-valued and continuous, except possibly at a finite number of finite discontinuities;
(iii) it must have only a finite number of maxima and minima within one period;
(iv) the integral over one period of $|f(x)|$ must converge.

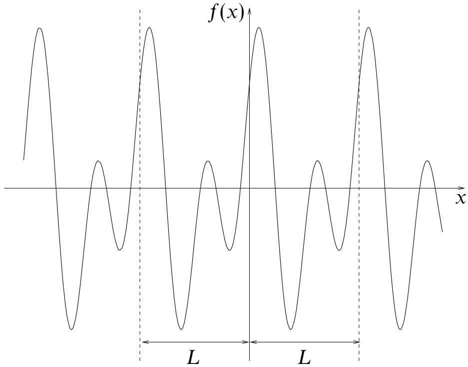

Figure 12.1 An example of a function that may be represented as a Fourier series without modification.

If the above conditions are satisfied then the Fourier series converges to $f(x)$ at all points where $f(x)$ is continuous. The convergence of the Fourier series at points of discontinuity is discussed in section 12.4. The last three Dirichlet conditions are almost always met in real applications, but not all functions are periodic and hence do not fulfil the first condition. It may be possible, however, to represent a non-periodic function as a Fourier series by manipulation of the function into a periodic form. This is discussed in section 12.5. An example of a function that may, without modification, be represented as a Fourier series is shown in figure 12.1.

We have stated without proof that any function that satisfies the Dirichlet conditions may be represented as a Fourier series. Let us now show why this is a plausible statement. We require that any reasonable function (one that satisfies the Dirichlet conditions) can be expressed as a linear sum of sine and cosine terms. We first note that we cannot use just a sum of sine terms since sine, being an odd function (i.e. a function for which $f(-x) = -f(x)$), cannot represent even functions (i.e. functions for which $f(-x) = f(x)$). This is obvious when we try to express a function $f(x)$ that takes a non-zero value at $x = 0$. Clearly, since $\sin nx = 0$ for all values of n, we cannot represent $f(x)$ at $x = 0$ by a sine series. Similarly odd functions cannot be represented by a cosine series since cosine is an even function. Nevertheless, it is possible to represent *all* odd functions by a sine series and *all* even functions by a cosine series. Now, since all functions may be written as the sum of an odd and an even part,

$$\begin{aligned} f(x) &= \tfrac{1}{2}[f(x) + f(-x)] + \tfrac{1}{2}[f(x) - f(-x)] \\ &= f_{\text{even}}(x) + f_{\text{odd}}(x), \end{aligned}$$

we can write any function as the sum of a sine series and a cosine series.

All the terms of a Fourier series are mutually orthogonal, i.e. the integrals, over one period, of the product of any two terms have the following properties:

$$\int_{x_0}^{x_0+L} \sin\left(\frac{2\pi rx}{L}\right) \cos\left(\frac{2\pi px}{L}\right) dx = 0 \quad \text{for all } r \text{ and } p, \tag{12.1}$$

$$\int_{x_0}^{x_0+L} \cos\left(\frac{2\pi rx}{L}\right) \cos\left(\frac{2\pi px}{L}\right) dx = \begin{cases} L & \text{for } r = p = 0, \\ \frac{1}{2}L & \text{for } r = p > 0, \\ 0 & \text{for } r \neq p, \end{cases} \tag{12.2}$$

$$\int_{x_0}^{x_0+L} \sin\left(\frac{2\pi rx}{L}\right) \sin\left(\frac{2\pi px}{L}\right) dx = \begin{cases} 0 & \text{for } r = p = 0, \\ \frac{1}{2}L & \text{for } r = p > 0, \\ 0 & \text{for } r \neq p, \end{cases} \tag{12.3}$$

where r and p are integers greater than or equal to zero; these formulae are easily derived. A full discussion of why it is possible to expand a function as a sum of mutually orthogonal functions is given in chapter 17.

The Fourier series expansion of the function $f(x)$ is conventionally written

$$f(x) = \frac{a_0}{2} + \sum_{r=1}^{\infty} \left[a_r \cos\left(\frac{2\pi rx}{L}\right) + b_r \sin\left(\frac{2\pi rx}{L}\right) \right], \tag{12.4}$$

where a_0, a_r, b_r are constants called the *Fourier coefficients*. These coefficients are analogous to those in a power series expansion and the determination of their numerical values is the essential step in writing a function as a Fourier series.

This chapter continues with a discussion of how to find the Fourier coefficients for particular functions. We then discuss simplifications to the general Fourier series that may save considerable effort in calculations. This is followed by the alternative representation of a function as a complex Fourier series, and we conclude with a discussion of Parseval's theorem.

12.2 The Fourier coefficients

We have indicated that a series that satisfies the Dirichlet conditions may be written in the form (12.4). We now consider how to find the Fourier coefficients for any particular function. For a periodic function $f(x)$ of period L we will find that the Fourier coefficients are given by

$$a_r = \frac{2}{L} \int_{x_0}^{x_0+L} f(x) \cos\left(\frac{2\pi rx}{L}\right) dx, \tag{12.5}$$

$$b_r = \frac{2}{L} \int_{x_0}^{x_0+L} f(x) \sin\left(\frac{2\pi rx}{L}\right) dx, \tag{12.6}$$

where x_0 is arbitrary but is often taken as 0 or $-L/2$. The apparently arbitrary factor $\frac{1}{2}$ which appears in the a_0 term in (12.4) is included so that (12.5) may apply for $r = 0$ as well as $r > 0$. The relations (12.5) and (12.6) may be derived as follows.

Suppose the Fourier series expansion of $f(x)$ can be written as in (12.4),

$$f(x) = \frac{a_0}{2} + \sum_{r=1}^{\infty} \left[a_r \cos\left(\frac{2\pi rx}{L}\right) + b_r \sin\left(\frac{2\pi rx}{L}\right) \right].$$

Then, multiplying by $\cos(2\pi px/L)$, integrating over one full period in x and changing the order of the summation and integration, we get

$$\begin{aligned} \int_{x_0}^{x_0+L} f(x) \cos\left(\frac{2\pi px}{L}\right) dx = {} & \frac{a_0}{2} \int_{x_0}^{x_0+L} \cos\left(\frac{2\pi px}{L}\right) dx \\ & + \sum_{r=1}^{\infty} a_r \int_{x_0}^{x_0+L} \cos\left(\frac{2\pi rx}{L}\right) \cos\left(\frac{2\pi px}{L}\right) dx \\ & + \sum_{r=1}^{\infty} b_r \int_{x_0}^{x_0+L} \sin\left(\frac{2\pi rx}{L}\right) \cos\left(\frac{2\pi px}{L}\right) dx. \end{aligned} \tag{12.7}$$

We can now find the Fourier coefficients by considering (12.7) as p takes different values. Using the orthogonality conditions (12.1)–(12.3) of the previous section, we find that when $p = 0$ (12.7) becomes

$$\int_{x_0}^{x_0+L} f(x)dx = \frac{a_0}{2} L.$$

When $p \neq 0$ the only non-vanishing term on the RHS of (12.7) occurs when $r = p$, and so

$$\int_{x_0}^{x_0+L} f(x) \cos\left(\frac{2\pi rx}{L}\right) dx = \frac{a_r}{2} L.$$

The other Fourier coefficients b_r may be found by repeating the above process but multiplying by $\sin(2\pi px/L)$ instead of $\cos(2\pi px/L)$ (see exercise 12.2).

►*Express the square-wave function illustrated in figure 12.2 as a Fourier series.*

Physically this might represent the input to an electrical circuit that switches between a high and a low state with time period T. The square wave may be represented by

$$f(t) = \begin{cases} -1 & \text{for } -\frac{1}{2}T \leq t < 0, \\ +1 & \text{for } 0 \leq t < \frac{1}{2}T. \end{cases}$$

In deriving the Fourier coefficients, we note firstly that the function is an odd function and so the series will contain only sine terms (this simplification is discussed further in the

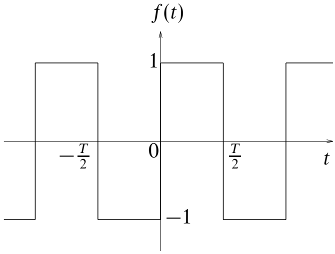

Figure 12.2 A square-wave function.

following section). To evaluate the coefficients in the sine series we use (12.6). Hence

$$\begin{aligned} b_r &= \frac{2}{T}\int_{-T/2}^{T/2} f(t)\sin\left(\frac{2\pi r t}{T}\right)\,dt \\ &= \frac{4}{T}\int_{0}^{T/2} \sin\left(\frac{2\pi r t}{T}\right)\,dt \\ &= \frac{2}{\pi r}\,[1-(-1)^r]\,. \end{aligned}$$

Thus the sine coefficients are zero if r is even and equal to $4/(\pi r)$ if r is odd. Hence the Fourier series for the square-wave function may be written as

$$f(t) = \frac{4}{\pi}\left(\sin\omega t + \frac{\sin 3\omega t}{3} + \frac{\sin 5\omega t}{5} + \cdots\right), \tag{12.8}$$

where $\omega = 2\pi/T$ is called the *angular frequency*. ◄

12.3 Symmetry considerations

The example in the previous section employed the useful property that since the function to be represented was odd, all the cosine terms of the Fourier series were absent. It is often the case that the function we wish to express as a Fourier series has a particular symmetry, which we can exploit to reduce the calculational labour of evaluating Fourier coefficients. Functions that are symmetric or antisymmetric about the origin (i.e. even and odd functions respectively) admit particularly useful simplifications. Functions that are odd in x have no cosine terms (see section 12.1) and all the a-coefficients are equal to zero. Similarly, functions that are even in x have no sine terms and all the b-coefficients are zero. Since the Fourier series of odd or even functions contain only half the coefficients required for a general periodic function, there is a considerable reduction in the algebra needed to find a Fourier series.

The consequences of symmetry or antisymmetry of the function about the quarter period (i.e. about $L/4$) are a little less obvious. Furthermore, the results are not used as often as those above and the remainder of this section can be omitted on a first reading without loss of continuity. The following argument gives the required results.

Suppose that $f(x)$ has even or odd symmetry about $L/4$, i.e. $f(L/4 - x) = \pm f(x - L/4)$. For convenience, we make the substitution $s = x - L/4$ and hence $f(-s) = \pm f(s)$. We can now see that

$$b_r = \frac{2}{L}\int_{x_0}^{x_0+L} f(s)\sin\left(\frac{2\pi rs}{L} + \frac{\pi r}{2}\right) ds,$$

where the limits of integration have been left unaltered since f is, of course, periodic in s as well as in x. If we use the expansion

$$\sin\left(\frac{2\pi rs}{L} + \frac{\pi r}{2}\right) = \sin\left(\frac{2\pi rs}{L}\right)\cos\left(\frac{\pi r}{2}\right) + \cos\left(\frac{2\pi rs}{L}\right)\sin\left(\frac{\pi r}{2}\right),$$

we can immediately see that the trigonometric part of the integrand is an odd function of s if r is even and an even function of s if r is odd. Hence if $f(s)$ is even and r is even then the integral is zero, and if $f(s)$ is odd and r is odd then the integral is zero. Similar results can be derived for the Fourier a-coefficients and we conclude that

(i) if $f(x)$ is even about $L/4$ then $a_{2r+1} = 0$ and $b_{2r} = 0$,
(ii) if $f(x)$ is odd about $L/4$ then $a_{2r} = 0$ and $b_{2r+1} = 0$.

All the above results follow automatically when the Fourier coefficients are evaluated in any particular case, but prior knowledge of them will often enable some coefficients to be set equal to zero on inspection and so substantially reduce the computational labour. As an example, the square-wave function shown in figure 12.2 is (i) an odd function of t, so that all $a_r = 0$, and (ii) even about the point $t = T/4$, so that $b_{2r} = 0$. Thus we can say immediately that only sine terms of odd harmonics will be present and therefore will need to be calculated; this is confirmed in the expansion (12.8).

12.4 Discontinuous functions

The Fourier series expansion usually works well for functions that are discontinuous in the required range. However, the series itself does not produce a discontinuous function and we state without proof that the value of the expanded $f(x)$ at a discontinuity will be half-way between the upper and lower values. Expressing this more mathematically, at a point of finite discontinuity, x_d, the Fourier series converges to

$$\tfrac{1}{2}\lim_{\epsilon\to 0}[f(x_d + \epsilon) + f(x_d - \epsilon)].$$

At a discontinuity, the Fourier series representation of the function will overshoot its value. Although as more terms are included the overshoot moves in position

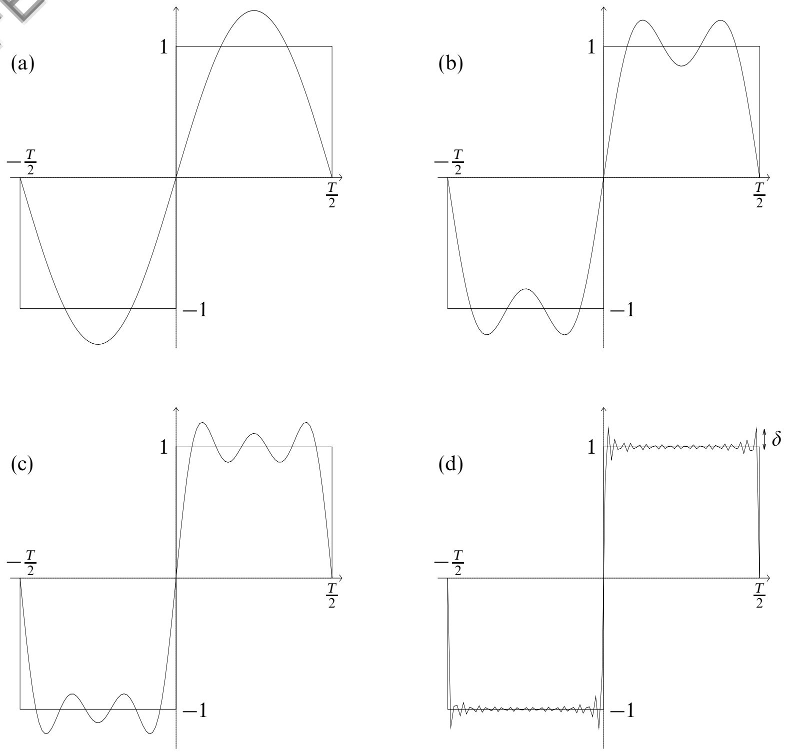

Figure 12.3 The convergence of a Fourier series expansion of a square-wave function, including (a) one term, (b) two terms, (c) three terms and (d) 20 terms. The overshoot δ is shown in (d).

arbitrarily close to the discontinuity, it never disappears even in the limit of an infinite number of terms. This behaviour is known as *Gibbs' phenomenon.* A full discussion is not pursued here but suffice it to say that the size of the overshoot is proportional to the magnitude of the discontinuity.

►*Find the value to which the Fourier series of the square-wave function discussed in section 12.2 converges at $t = 0$.*

It can be seen that the function is discontinuous at $t = 0$ and, by the above rule, we expect the series to converge to a value half-way between the upper and lower values, in other words to converge to zero in this case. Considering the Fourier series of this function, (12.8), we see that all the terms are zero and hence the Fourier series converges to zero as expected. The Gibbs phenomenon for the square-wave function is shown in figure 12.3. ◄

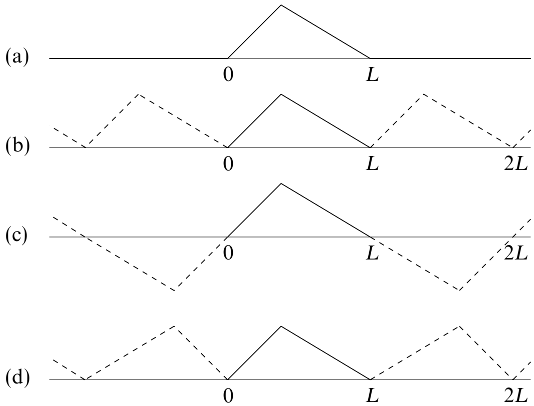

Figure 12.4 Possible periodic extensions of a function.

12.5 Non-periodic functions

We have already mentioned that a Fourier representation may sometimes be used for non-periodic functions. If we wish to find the Fourier series of a non-periodic function only within a fixed range then we may *continue* the function outside the range so as to make it periodic. The Fourier series of this periodic function would then correctly represent the non-periodic function in the desired range. Since we are often at liberty to extend the function in a number of ways, we can sometimes make it odd or even and so reduce the calculation required. Figure 12.4(b) shows the simplest extension to the function shown in figure 12.4(a). However, this extension has no particular symmetry. Figures 12.4(c), (d) show extensions as odd and even functions respectively with the benefit that only sine or cosine terms appear in the resulting Fourier series. We note that these last two extensions give a function of period $2L$.

In view of the result of section 12.4, it must be added that the continuation must not be discontinuous at the end-points of the interval of interest; if it is the series will not converge to the required value there. This requirement that the series converges appropriately may reduce the choice of continuations. This is discussed further at the end of the following example.

►*Find the Fourier series of* $f(x) = x^2$ *for* $0 < x \leq 2$.

We must first make the function periodic. We do this by extending the range of interest to $-2 < x \leq 2$ in such a way that $f(x) = f(-x)$ and then letting $f(x + 4k) = f(x)$, where k is any integer. This is shown in figure 12.5. Now we have an even function of period 4. The Fourier series will faithfully represent $f(x)$ in the range, $-2 < x \leq 2$, although not outside it. Firstly we note that since we have made the specified function even in x by extending

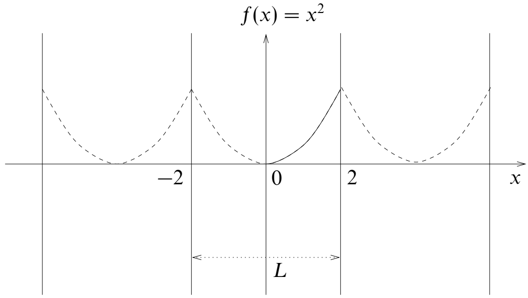

Figure 12.5 $f(x) = x^2$, $0 < x \le 2$, with the range extended to give periodicity.

the range, all the coefficients b_r will be zero. Now we apply (12.5) and (12.6) with $L = 4$ to determine the remaining coefficients:

$$a_r = \frac{2}{4}\int_{-2}^{2} x^2 \cos\left(\frac{2\pi r x}{4}\right) dx = \frac{4}{4}\int_0^2 x^2 \cos\left(\frac{\pi r x}{2}\right) dx,$$

where the second equality holds because the function is even in x. Thus

$$\begin{aligned} a_r &= \left[\frac{2}{\pi r}x^2 \sin\left(\frac{\pi r x}{2}\right)\right]_0^2 - \frac{4}{\pi r}\int_0^2 x \sin\left(\frac{\pi r x}{2}\right) dx \\ &= \frac{8}{\pi^2 r^2}\left[x \cos\left(\frac{\pi r x}{2}\right)\right]_0^2 - \frac{8}{\pi^2 r^2}\int_0^2 \cos\left(\frac{\pi r x}{2}\right) dx \\ &= \frac{16}{\pi^2 r^2}\cos \pi r \\ &= \frac{16}{\pi^2 r^2}(-1)^r. \end{aligned}$$

Since this expression for a_r has r^2 in its denominator, to evaluate a_0 we must return to the original definition,

$$a_r = \frac{2}{4}\int_{-2}^{2} f(x) \cos\left(\frac{\pi r x}{2}\right) dx.$$

From this we obtain

$$a_0 = \frac{2}{4}\int_{-2}^{2} x^2\, dx = \frac{4}{4}\int_0^2 x^2\, dx = \frac{8}{3}.$$

The final expression for $f(x)$ is then

$$x^2 = \frac{4}{3} + 16\sum_{r=1}^{\infty} \frac{(-1)^r}{\pi^2 r^2} \cos\left(\frac{\pi r x}{2}\right) \qquad \text{for } 0 < x \le 2. ◀$$

We note that in the above example we could have extended the range so as to make the function odd. In other words we could have set $f(x) = -f(-x)$ and then made $f(x)$ periodic in such a way that $f(x + 4) = f(x)$. In this case the resulting Fourier series would be a series of just sine terms. However, although this will faithfully represent the function inside the required range, it does not converge to the correct values of $f(x) = \pm 4$ at $x = \pm 2$; it converges, instead, to zero, the average of the values at the two ends of the range.

12.6 Integration and differentiation

It is sometimes possible to find the Fourier series of a function by integration or differentiation of another Fourier series. If the Fourier series of $f(x)$ is integrated term by term then the resulting Fourier series converges to the integral of $f(x)$. Clearly, when integrating in such a way there is a constant of integration that must be found. If $f(x)$ is a continuous function of x for all x and $f(x)$ is also periodic then the Fourier series that results from differentiating term by term converges to $f'(x)$, provided that $f'(x)$ itself satisfies the Dirichlet conditions. These properties of Fourier series may be useful in calculating complicated Fourier series, since simple Fourier series may easily be evaluated (or found from standard tables) and often the more complicated series can then be built up by integration and/or differentiation.

►*Find the Fourier series of* $f(x) = x^3$ *for* $0 < x \leq 2$.

In the example discussed in the previous section we found the Fourier series for $f(x) = x^2$ in the required range. So, if we *integrate* this term by term, we obtain

$$\frac{x^3}{3} = \frac{4}{3}x + 32\sum_{r=1}^{\infty} \frac{(-1)^r}{\pi^3 r^3} \sin\left(\frac{\pi r x}{2}\right) + c,$$

where c is, so far, an arbitrary constant. We have not yet found the Fourier series for x^3 because the term $\frac{4}{3}x$ appears in the expansion. However, by now *differentiating* the same initial expression for x^2 we obtain

$$2x = -8\sum_{r=1}^{\infty} \frac{(-1)^r}{\pi r} \sin\left(\frac{\pi r x}{2}\right).$$

We can now write the full Fourier expansion of x^3 as

$$x^3 = -16\sum_{r=1}^{\infty} \frac{(-1)^r}{\pi r} \sin\left(\frac{\pi r x}{2}\right) + 96\sum_{r=1}^{\infty} \frac{(-1)^r}{\pi^3 r^3} \sin\left(\frac{\pi r x}{2}\right) + c.$$

Finally, we can find the constant, c, by considering $f(0)$. At $x = 0$, our Fourier expansion gives $x^3 = c$ since all the sine terms are zero, and hence $c = 0$. ◄

12.7 Complex Fourier series

As a Fourier series expansion in general contains both sine and cosine parts, it may be written more compactly using a complex exponential expansion. This simplification makes use of the property that $\exp(irx) = \cos rx + i \sin rx$. The complex Fourier series expansion is written

$$f(x) = \sum_{r=-\infty}^{\infty} c_r \exp\left(\frac{2\pi i r x}{L}\right), \qquad (12.9)$$

where the Fourier coefficients are given by

$$c_r = \frac{1}{L}\int_{x_0}^{x_0+L} f(x) \exp\left(-\frac{2\pi irx}{L}\right) dx. \tag{12.10}$$

This relation can be derived, in a similar manner to that of section 12.2, by multiplying (12.9) by $\exp(-2\pi ipx/L)$ before integrating and using the orthogonality relation

$$\int_{x_0}^{x_0+L} \exp\left(-\frac{2\pi ipx}{L}\right) \exp\left(\frac{2\pi irx}{L}\right) dx = \begin{cases} L & \text{for } r = p, \\ 0 & \text{for } r \neq p. \end{cases}$$

The complex Fourier coefficients in (12.9) have the following relations to the real Fourier coefficients:

$$\begin{aligned} c_r &= \tfrac{1}{2}(a_r - ib_r), \\ c_{-r} &= \tfrac{1}{2}(a_r + ib_r). \end{aligned} \tag{12.11}$$

Note that if $f(x)$ is real then $c_{-r} = c_r^*$, where the asterisk represents complex conjugation.

▶*Find a complex Fourier series for* $f(x) = x$ *in the range* $-2 < x < 2$.

Using (12.10), for $r \neq 0$,

$$\begin{aligned} c_r &= \frac{1}{4}\int_{-2}^{2} x \exp\left(-\frac{\pi irx}{2}\right) dx \\ &= \left[-\frac{x}{2\pi ir}\exp\left(-\frac{\pi irx}{2}\right)\right]_{-2}^{2} + \int_{-2}^{2} \frac{1}{2\pi ir}\exp\left(-\frac{\pi irx}{2}\right) dx \\ &= -\frac{1}{\pi ir}\left[\exp(-\pi ir) + \exp(\pi ir)\right] + \left[\frac{1}{r^2\pi^2}\exp\left(-\frac{\pi irx}{2}\right)\right]_{-2}^{2} \\ &= \frac{2i}{\pi r}\cos \pi r - \frac{2i}{r^2\pi^2}\sin \pi r = \frac{2i}{\pi r}(-1)^r. \end{aligned} \tag{12.12}$$

For $r = 0$, we find $c_0 = 0$ and hence

$$x = \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \frac{2i(-1)^r}{r\pi} \exp\left(\frac{\pi irx}{2}\right).$$

We note that the Fourier series derived for x in section 12.6 gives $a_r = 0$ for all r and

$$b_r = -\frac{4(-1)^r}{\pi r},$$

and so, using (12.11), we confirm that c_r and c_{-r} have the forms derived above. It is also apparent that the relationship $c_r^* = c_{-r}$ holds, as we expect since $f(x)$ is real. ◀

12.8 Parseval's theorem

Parseval's theorem gives a useful way of relating the Fourier coefficients to the function that they describe. Essentially a conservation law, it states that

$$\frac{1}{L}\int_{x_0}^{x_0+L} |f(x)|^2 dx = \sum_{r=-\infty}^{\infty} |c_r|^2$$

$$= \left(\tfrac{1}{2}a_0\right)^2 + \tfrac{1}{2}\sum_{r=1}^{\infty}(a_r^2 + b_r^2). \qquad (12.13)$$

In a more memorable form, this says that the sum of the moduli squared of the complex Fourier coefficients is equal to the average value of $|f(x)|^2$ over one period. Parseval's theorem can be proved straightforwardly by writing $f(x)$ as a Fourier series and evaluating the required integral, but the algebra is messy. Therefore, we shall use an alternative method, for which the algebra is simple and which in fact leads to a more general form of the theorem.

Let us consider two functions $f(x)$ and $g(x)$, which are (or can be made) periodic with period L and which have Fourier series (expressed in complex form)

$$f(x) = \sum_{r=-\infty}^{\infty} c_r \exp\left(\frac{2\pi irx}{L}\right),$$

$$g(x) = \sum_{r=-\infty}^{\infty} \gamma_r \exp\left(\frac{2\pi irx}{L}\right),$$

where c_r and γ_r are the complex Fourier coefficients of $f(x)$ and $g(x)$ respectively. Thus

$$f(x)g^*(x) = \sum_{r=-\infty}^{\infty} c_r g^*(x) \exp\left(\frac{2\pi irx}{L}\right).$$

Integrating this equation with respect to x over the interval $(x_0, x_0 + L)$ and dividing by L, we find

$$\frac{1}{L}\int_{x_0}^{x_0+L} f(x)g^*(x)\,dx = \sum_{r=-\infty}^{\infty} c_r \frac{1}{L}\int_{x_0}^{x_0+L} g^*(x)\exp\left(\frac{2\pi irx}{L}\right)dx$$

$$= \sum_{r=-\infty}^{\infty} c_r \left[\frac{1}{L}\int_{x_0}^{x_0+L} g(x)\exp\left(\frac{-2\pi irx}{L}\right)dx\right]^*$$

$$= \sum_{r=-\infty}^{\infty} c_r \gamma_r^*,$$

where the last equality uses (12.10). Finally, if we let $g(x) = f(x)$ then we obtain Parseval's theorem (12.13). This result can be proved in a similar manner using the sine and cosine form of the Fourier series, but the algebra is slightly more complicated.

Parseval's theorem is sometimes used to sum series. However, if one is presented with a series to sum, it is not usually possible to decide which Fourier series should be used to evaluate it. Rather, useful summations are nearly always found serendipitously. The following example shows the evaluation of a sum by a Fourier series method.

►*Using Parseval's theorem and the Fourier series for $f(x) = x^2$ found in section 12.5, calculate the sum $\sum_{r=1}^{\infty} r^{-4}$.*

Firstly we find the average value of $[f(x)]^2$ over the interval $-2 < x \le 2$:

$$\frac{1}{4}\int_{-2}^{2} x^4\,dx = \frac{16}{5}.$$

Now we evaluate the right-hand side of (12.13):

$$\left(\tfrac{1}{2}a_0\right)^2 + \tfrac{1}{2}\sum_{1}^{\infty} a_r^2 + \tfrac{1}{2}\sum_{1}^{\infty} b_n^2 = \left(\tfrac{4}{3}\right)^2 + \tfrac{1}{2}\sum_{r=1}^{\infty}\frac{16^2}{\pi^4 r^4}.$$

Equating the two expression we find

$$\sum_{r=1}^{\infty}\frac{1}{r^4} = \frac{\pi^4}{90}. \blacktriangleleft$$

12.9 Exercises

12.1 Prove the orthogonality relations stated in section 12.1.

12.2 Derive the Fourier coefficients b_r in a similar manner to the derivation of the a_r in section 12.2.

12.3 Which of the following functions of x could be represented by a Fourier series over the range indicated?

(a) $\tanh^{-1}(x)$, $\quad -\infty < x < \infty$;
(b) $\tan x$, $\quad -\infty < x < \infty$;
(c) $|\sin x|^{-1/2}$, $\quad -\infty < x < \infty$;
(d) $\cos^{-1}(\sin 2x)$, $\quad -\infty < x < \infty$;
(e) $x\sin(1/x)$, $\quad -\pi^{-1} < x \le \pi^{-1}$, cyclically repeated.

12.4 By moving the origin of t to the centre of an interval in which $f(t) = +1$, i.e. by changing to a new independent variable $t' = t - \frac{1}{4}T$, express the square-wave function in the example in section 12.2 as a cosine series. Calculate the Fourier coefficients involved (a) directly and (b) by changing the variable in result (12.8).

12.5 Find the Fourier series of the function $f(x) = x$ in the range $-\pi < x \le \pi$. Hence show that

$$1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \cdots = \frac{\pi}{4}.$$

12.6 For the function

$$f(x) = 1 - x, \qquad 0 \le x \le 1,$$

find (a) the Fourier sine series and (b) the Fourier cosine series. Which would be better for numerical evaluation? Relate your answer to the relevant periodic continuations.

12.7 For the continued functions used in exercise 12.6 and the derived corresponding series, consider (i) their derivatives and (ii) their integrals. Do they give meaningful equations? You will probably find it helpful to sketch all the functions involved.

12.8 The function $y(x) = x \sin x$ for $0 \le x \le \pi$ is to be represented by a Fourier series of period 2π that is either even or odd. By sketching the function and considering its derivative, determine which series will have the more rapid convergence. Find the full expression for the better of these two series, showing that the convergence $\sim n^{-3}$ and that alternate terms are missing.

12.9 Find the Fourier coefficients in the expansion of $f(x) = \exp x$ over the range $-1 < x < 1$. What value will the expansion have when $x = 2$?

12.10 By integrating term by term the Fourier series found in the previous question and using the Fourier series for $f(x) = x$ found in section 12.6, show that $\int \exp x \, dx = \exp x + c$. Why is it not possible to show that $d(\exp x)/dx = \exp x$ by differentiating the Fourier series of $f(x) = \exp x$ in a similar manner?

12.11 Consider the function $f(x) = \exp(-x^2)$ in the range $0 \le x \le 1$. Show how it should be continued to give as its Fourier series a series (the actual form is not wanted) (a) with only cosine terms, (b) with only sine terms, (c) with period 1 and (d) with period 2.

Would there be any difference between the values of the last two series at (i) $x = 0$, (ii) $x = 1$?

12.12 Find, without calculation, which terms will be present in the Fourier series for the periodic functions $f(t)$, of period T, that are given in the range $-T/2$ to $T/2$ by:

(a) $f(t) = 2$ for $0 \le |t| < T/4$, $f = 1$ for $T/4 \le |t| < T/2$;
(b) $f(t) = \exp[-(t - T/4)^2]$;
(c) $f(t) = -1$ for $-T/2 \le t < -3T/8$ and $3T/8 \le t < T/2, f(t) = 1$ for $-T/8 \le t < T/8$; the graph of f is completed by two straight lines in the remaining ranges so as to form a continuous function.

12.13 Consider the representation as a Fourier series of the displacement of a string lying in the interval $0 \le x \le L$ and fixed at its ends, when it is pulled aside by y_0 at the point $x = L/4$. Sketch the continuations for the region outside the interval that will

(a) produce a series of period L,
(b) produce a series that is antisymmetric about $x = 0$, and
(c) produce a series that will contain only cosine terms.
(d) What are (i) the periods of the series in (b) and (c) and (ii) the value of the 'a_0-term' in (c)?
(e) Show that a typical term of the series obtained in (b) is

$$\frac{32y_0}{3n^2\pi^2} \sin \frac{n\pi}{4} \sin \frac{n\pi x}{L}.$$

12.14 Show that the Fourier series for the function $y(x) = |x|$ in the range $-\pi \le x < \pi$ is

$$y(x) = \frac{\pi}{2} - \frac{4}{\pi} \sum_{m=0}^{\infty} \frac{\cos(2m+1)x}{(2m+1)^2}.$$

By integrating this equation term by term from 0 to x, find the function $g(x)$ whose Fourier series is

$$\frac{4}{\pi} \sum_{m=0}^{\infty} \frac{\sin(2m+1)x}{(2m+1)^3}.$$

Deduce the value of the sum S of the series

$$1 - \frac{1}{3^3} + \frac{1}{5^3} - \frac{1}{7^3} + \cdots.$$

12.15 Using the result of exercise 12.14, determine, as far as possible by inspection, the forms of the functions of which the following are the Fourier series:

(a)

$$\cos\theta + \frac{1}{9}\cos 3\theta + \frac{1}{25}\cos 5\theta + \cdots ;$$

(b)

$$\sin\theta + \frac{1}{27}\sin 3\theta + \frac{1}{125}\sin 5\theta + \cdots ;$$

(c)

$$\frac{L^2}{3} - \frac{4L^2}{\pi^2}\left[\cos\frac{\pi x}{L} - \frac{1}{4}\cos\frac{2\pi x}{L} + \frac{1}{9}\cos\frac{3\pi x}{L} - \cdots\right].$$

(You may find it helpful to first set $x = 0$ in the quoted result and so obtain values for $S_o = \sum(2m+1)^{-2}$ and other sums derivable from it.)

12.16 By finding a cosine Fourier series of period 2 for the function $f(t)$ that takes the form $f(t) = \cosh(t-1)$ in the range $0 \le t \le 1$, prove that

$$\sum_{n=1}^{\infty} \frac{1}{n^2\pi^2 + 1} = \frac{1}{e^2 - 1}.$$

Deduce values for the sums $\sum(n^2\pi^2 + 1)^{-1}$ over odd n and even n separately.

12.17 Find the (real) Fourier series of period 2 for $f(x) = \cosh x$ and $g(x) = x^2$ in the range $-1 \le x \le 1$. By integrating the series for $f(x)$ twice, prove that

$$\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^2\pi^2(n^2\pi^2+1)} = \frac{1}{2}\left(\frac{1}{\sinh 1} - \frac{5}{6}\right).$$

12.18 Express the function $f(x) = x^2$ as a Fourier sine series in the range $0 < x \le 2$ and show that it converges to zero at $x = \pm 2$.

12.19 Demonstrate explicitly for the square-wave function discussed in section 12.2 that Parseval's theorem (12.13) is valid. You will need to use the relationship

$$\sum_{m=0}^{\infty} \frac{1}{(2m+1)^2} = \frac{\pi^2}{8}.$$

Show that a filter that transmits frequencies only up to $8\pi/T$ will still transmit more than 90% of the power in such a square-wave voltage signal.

12.20 Show that the Fourier series for $|\sin\theta|$ in the range $-\pi \le \theta \le \pi$ is given by

$$|\sin\theta| = \frac{2}{\pi} - \frac{4}{\pi}\sum_{m=1}^{\infty} \frac{\cos 2m\theta}{4m^2 - 1}.$$

By setting $\theta = 0$ and $\theta = \pi/2$, deduce values for

$$\sum_{m=1}^{\infty} \frac{1}{4m^2 - 1} \quad \text{and} \quad \sum_{m=1}^{\infty} \frac{1}{16m^2 - 1}.$$

12.21 Find the complex Fourier series for the periodic function of period 2π defined in the range $-\pi \le x \le \pi$ by $y(x) = \cosh x$. By setting $x = 0$ prove that

$$\sum_{n=1}^{\infty} \frac{(-1)^n}{n^2+1} = \frac{1}{2}\left(\frac{\pi}{\sinh \pi} - 1\right).$$

12.22 The repeating output from an electronic oscillator takes the form of a sine wave $f(t) = \sin t$ for $0 \le t \le \pi/2$; it then drops instantaneously to zero and starts again. The output is to be represented by a complex Fourier series of the form

$$\sum_{n=-\infty}^{\infty} c_n e^{4nti}.$$

Sketch the function and find an expression for c_n. Verify that $c_{-n} = c_n^*$. Demonstrate that setting $t = 0$ and $t = \pi/2$ produces differing values for the sum

$$\sum_{n=1}^{\infty} \frac{1}{16n^2 - 1}.$$

Determine the correct value and check it using the result of exercise 12.20.

12.23 Apply Parseval's theorem to the series found in the previous exercise and so derive a value for the sum of the series

$$\frac{17}{(15)^2} + \frac{65}{(63)^2} + \frac{145}{(143)^2} + \cdots + \frac{16n^2+1}{(16n^2-1)^2} + \cdots.$$

12.24 A string, anchored at $x = \pm L/2$, has a fundamental vibration frequency of $2L/c$, where c is the speed of transverse waves on the string. It is pulled aside at its centre point by a distance y_0 and released at time $t = 0$. Its subsequent motion can be described by the series

$$y(x,t) = \sum_{n=1}^{\infty} a_n \cos\frac{n\pi x}{L} \cos\frac{n\pi ct}{L}.$$

Find a general expression for a_n and show that only the odd harmonics of the fundamental frequency are present in the sound generated by the released string. By applying Parseval's theorem, find the sum S of the series $\sum_0^{\infty}(2m+1)^{-4}$.

12.25 Show that Parseval's theorem for two real functions whose Fourier expansions have cosine and sine coefficients a_n, b_n and α_n, β_n takes the form

$$\frac{1}{L}\int_0^L f(x)g^*(x)\,dx = \frac{1}{4}a_0\alpha_0 + \frac{1}{2}\sum_{n=1}^{\infty}(a_n\alpha_n + b_n\beta_n).$$

(a) Demonstrate that for $g(x) = \sin mx$ or $\cos mx$ this reduces to the definition of the Fourier coefficients.

(b) Explicitly verify the above result for the case in which $f(x) = x$ and $g(x)$ is the square-wave function, both in the interval $-1 \le x \le 1$.

12.26 An odd function $f(x)$ of period 2π is to be approximated by a Fourier sine series having only m terms. The error in this approximation is measured by the square deviation

$$E_m = \int_{-\pi}^{\pi}\left[f(x) - \sum_{n=1}^{m} b_n \sin nx\right]^2 dx.$$

By differentiating E_m with respect to the coefficients b_n, find the values of b_n that minimise E_m.

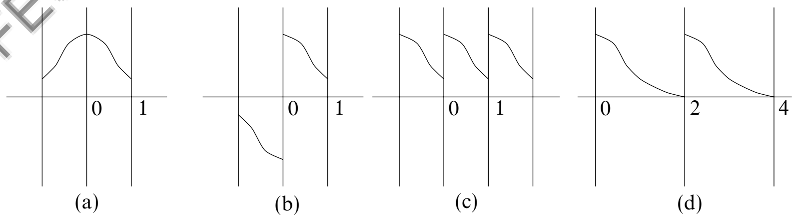

Figure 12.6 Continuations of $\exp(-x^2)$ in $0 \le x \le 1$ to give: (a) cosine terms only; (b) sine terms only; (c) period 1; (d) period 2.

Sketch the graph of the function $f(x)$, where

$$f(x) = \begin{cases} -x(\pi + x) & \text{for } -\pi \le x < 0, \\ x(x - \pi) & \text{for } 0 \le x < \pi. \end{cases}$$

If $f(x)$ is to be approximated by the first three terms of a Fourier sine series, what values should the coefficients have so as to minimise E_3? What is the resulting value of E_3?

12.10 Hints and answers

12.1 Note that the only integral of a sinusoid around a complete cycle of length L that is not zero is the integral of $\cos(2\pi nx/L)$ when $n = 0$.

12.3 Only (c). In terms of the Dirichlet conditions (section 12.1), the others fail as follows: (a) (i); (b) (ii); (d) (ii); (e) (iii).

12.5 $f(x) = 2\sum_1^\infty (-1)^{n+1} n^{-1} \sin nx$; set $x = \pi/2$.

12.7 (i) Series (a) from exercise 12.6 does not converge and cannot represent the function $y(x) = -1$. Series (b) reproduces the square-wave function of equation (12.8).
(ii) Series (a) gives the series for $y(x) = -x - \frac{1}{2}x^2 - \frac{1}{2}$ in the range $-1 \le x \le 0$ and for $y(x) = x - \frac{1}{2}x^2 - \frac{1}{2}$ in the range $0 \le x \le 1$. Series (b) gives the series for $y(x) = x + \frac{1}{2}x^2 + \frac{1}{2}$ in the range $-1 \le x \le 0$ and for $y(x) = x - \frac{1}{2}x^2 + \frac{1}{2}$ in the range $0 \le x \le 1$.

12.9 $f(x) = (\sinh 1)\left\{1 + 2\sum_1^\infty (-1)^n (1 + n^2\pi^2)^{-1} [\cos(n\pi x) - n\pi \sin(n\pi x)]\right\}$.
The series will converge to the same value as it does at $x = 0$, i.e. $f(0) = 1$.

12.11 See figure 12.6. (c) (i) $(1 + e^{-1})/2$, (ii) $(1 + e^{-1})/2$; (d) (i) $(1 + e^{-4})/2$, (ii) e^{-1}.

12.13 (d) (i) The periods are both $2L$; (ii) $y_0/2$.

12.15 $S_o = \pi^2/8$. If $S_e = \sum (2m)^{-2}$ then $S_e = \frac{1}{4}(S_e + S_o)$, yielding $S_o - S_e = \pi^2/12$ and $S_e + S_o = \pi^2/6$.
(a) $(\pi/4)(\pi/2 - |\theta|)$; (b) $(\pi\theta/4)(\pi/2 - |\theta|/2)$ from integrating (a). (c) Even function; average value $L^2/3$; $y(0) = 0$; $y(L) = L^2$; probably $y(x) = x^2$. Compare with the worked example in section 12.5.

12.17 $\cosh x = (\sinh 1)[1 + 2\sum_{n=1}^\infty (-1)^n (\cos n\pi x)/(n^2\pi^2 + 1)]$ and after integrating twice this form must be recovered. Use $x^2 = \frac{1}{3} + 4\sum(-1)^n(\cos n\pi x)/(n^2\pi^2)]$ to eliminate the quadratic term arising from the constants of integration; there is no linear term.

12.19 $C_{\pm(2m+1)} = \mp 2i/[(2m+1)\pi]$; $\sum |C_n|^2 = (4/\pi^2) \times 2 \times (\pi^2/8)$; the values $n = \pm 1$, ± 3 contribute $> 90\%$ of the total.

12.21 $c_n = [(-1)^n \sinh \pi]/[\pi(1 + n^2)]$. Having set $x = 0$, separate out the $n = 0$ term and note that $(-1)^n = (-1)^{-n}$.

12.23 $(\pi^2 - 8)/16$.

12.25 (b) All a_n and α_n are zero; $b_n = 2(-1)^{n+1}/(n\pi)$ and $\beta_n = 4/(n\pi)$. You will need the result quoted in exercise 12.19.

13

Integral transforms

In the previous chapter we encountered the Fourier series representation of a periodic function in a fixed interval as a superposition of sinusoidal functions. It is often desirable, however, to obtain such a representation even for functions defined over an infinite interval and with no particular periodicity. Such a representation is called a *Fourier transform* and is one of a class of representations called *integral transforms*.

We begin by considering Fourier transforms as a generalisation of Fourier series. We then go on to discuss the properties of the Fourier transform and its applications. In the second part of the chapter we present an analogous discussion of the closely related *Laplace transform*.

13.1 Fourier transforms

The Fourier transform provides a representation of functions defined over an infinite interval and having no particular periodicity, in terms of a superposition of sinusoidal functions. It may thus be considered as a generalisation of the Fourier series representation of periodic functions. Since Fourier transforms are often used to represent time-varying functions, we shall present much of our discussion in terms of $f(t)$, rather than $f(x)$, although in some spatial examples $f(x)$ will be the more natural notation and we shall use it as appropriate. Our only requirement on $f(t)$ will be that $\int_{-\infty}^{\infty} |f(t)|\,dt$ is finite.

In order to develop the transition from Fourier series to Fourier transforms, we first recall that a function of period T may be represented as a complex Fourier series, cf. (12.9),

$$f(t) = \sum_{r=-\infty}^{\infty} c_r\, e^{2\pi irt/T} = \sum_{r=-\infty}^{\infty} c_r\, e^{i\omega_r t}, \tag{13.1}$$

where $\omega_r = 2\pi r/T$. As the period T tends to infinity, the ‘frequency quantum’

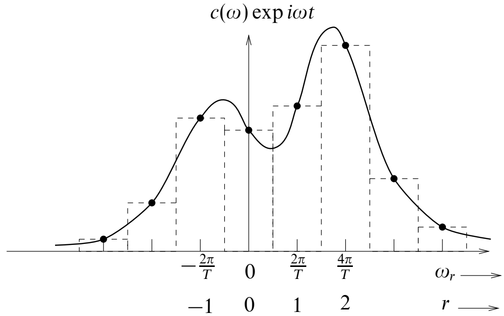

Figure 13.1 The relationship between the Fourier terms for a function of period T and the Fourier integral (the area below the solid line) of the function.

$\Delta\omega = 2\pi/T$ becomes vanishingly small and the spectrum of allowed frequencies ω_r becomes a continuum. Thus, the infinite sum of terms in the Fourier series becomes an integral, and the coefficients c_r become functions of the *continuous* variable ω, as follows.

We recall, cf. (12.10), that the coefficients c_r in (13.1) are given by

$$c_r = \frac{1}{T}\int_{-T/2}^{T/2} f(t)\, e^{-2\pi irt/T}\, dt = \frac{\Delta\omega}{2\pi}\int_{-T/2}^{T/2} f(t)\, e^{-i\omega_r t}\, dt, \tag{13.2}$$

where we have written the integral in two alternative forms and, for convenience, made one period run from $-T/2$ to $+T/2$ rather than from 0 to T. Substituting from (13.2) into (13.1) gives

$$f(t) = \sum_{r=-\infty}^{\infty} \frac{\Delta\omega}{2\pi}\int_{-T/2}^{T/2} f(u)\, e^{-i\omega_r u}\, du\; e^{i\omega_r t}. \tag{13.3}$$

At this stage ω_r is still a discrete function of r equal to $2\pi r/T$.

The solid points in figure 13.1 are a plot of (say, the real part of) $c_r\, e^{i\omega_r t}$ as a function of r (or equivalently of ω_r) and it is clear that $(2\pi/T)c_r\, e^{i\omega_r t}$ gives the area of the rth broken-line rectangle. If T tends to ∞ then $\Delta\omega$ $(= 2\pi/T)$ becomes infinitesimal, the width of the rectangles tends to zero and, from the mathematical definition of an integral,

$$\sum_{r=-\infty}^{\infty} \frac{\Delta\omega}{2\pi} g(\omega_r)\, e^{i\omega_r t} \quad\to\quad \frac{1}{2\pi}\int_{-\infty}^{\infty} g(\omega)\, e^{i\omega t}\, d\omega.$$

In this particular case

$$g(\omega_r) = \int_{-T/2}^{T/2} f(u)\, e^{-i\omega_r u}\, du,$$

and (13.3) becomes

$$f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{i\omega t}\int_{-\infty}^{\infty} du\, f(u)\, e^{-i\omega u}. \tag{13.4}$$

This result is known as *Fourier's inversion theorem.*

From it we may define the *Fourier transform* of $f(t)$ by

$$\widetilde{f}(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)\, e^{-i\omega t}\, dt, \tag{13.5}$$

and its inverse by

$$f(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \widetilde{f}(\omega)\, e^{i\omega t}\, d\omega. \tag{13.6}$$

Including the constant $1/\sqrt{2\pi}$ in the definition of $\widetilde{f}(\omega)$ (whose mathematical existence as $T \to \infty$ is assumed here without proof) is clearly arbitrary, the only requirement being that the product of the constants in (13.5) and (13.6) should equal $1/(2\pi)$. Our definition is chosen to be as symmetric as possible.

► *Find the Fourier transform of the exponential decay function $f(t) = 0$ for $t < 0$ and $f(t) = A\,e^{-\lambda t}$ for $t \geq 0$ $(\lambda > 0)$.*

Using the definition (13.5) and separating the integral into two parts,

$$\begin{aligned}
\widetilde{f}(\omega) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{0} (0)\, e^{-i\omega t}\, dt + \frac{A}{\sqrt{2\pi}}\int_{0}^{\infty} e^{-\lambda t}\, e^{-i\omega t}\, dt \\
&= 0 + \frac{A}{\sqrt{2\pi}}\left[-\frac{e^{-(\lambda+i\omega)t}}{\lambda + i\omega}\right]_0^{\infty} \\
&= \frac{A}{\sqrt{2\pi}(\lambda + i\omega)},
\end{aligned}$$

which is the required transform. It is clear that the multiplicative constant A does not affect the form of the transform, merely its amplitude. This transform may be verified by resubstitution of the above result into (13.6) to recover $f(t)$, but evaluation of the integral requires the use of complex-variable contour integration (chapter 24). ◄

13.1.1 The uncertainty principle

An important function that appears in many areas of physical science, either precisely or as an approximation to a physical situation, is the *Gaussian* or *normal* distribution. Its Fourier transform is of importance both in itself and also because, when interpreted statistically, it readily illustrates a form of *uncertainty principle.*

►*Find the Fourier transform of the normalised Gaussian distribution*

$$f(t) = \frac{1}{\tau\sqrt{2\pi}} \exp\left(-\frac{t^2}{2\tau^2}\right), \qquad -\infty < t < \infty.$$

This Gaussian distribution is centred on $t = 0$ and has a root mean square deviation $\Delta t = \tau$. (Any reader who is unfamiliar with this interpretation of the distribution should refer to chapter 30.)

Using the definition (13.5), the Fourier transform of $f(t)$ is given by

$$\begin{aligned}\widetilde{f}(\omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\tau\sqrt{2\pi}} \exp\left(-\frac{t^2}{2\tau^2}\right) \exp(-i\omega t)\, dt \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\tau\sqrt{2\pi}} \exp\left\{-\frac{1}{2\tau^2}\left[t^2 + 2\tau^2 i\omega t + (\tau^2 i\omega)^2 - (\tau^2 i\omega)^2\right]\right\} dt,\end{aligned}$$

where the quantity $-(\tau^2 i\omega)^2/(2\tau^2)$ has been both added and subtracted in the exponent in order to allow the factors involving the variable of integration t to be expressed as a complete square. Hence the expression can be written

$$\widetilde{f}(\omega) = \frac{\exp(-\frac{1}{2}\tau^2\omega^2)}{\sqrt{2\pi}} \left\{\frac{1}{\tau\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left[-\frac{(t + i\tau^2\omega)^2}{2\tau^2}\right] dt\right\}.$$

The quantity inside the braces is the normalisation integral for the Gaussian and equals unity, although to show this strictly needs results from complex variable theory (chapter 24). That it is equal to unity can be made plausible by changing the variable to $s = t + i\tau^2\omega$ and assuming that the imaginary parts introduced into the integration path and limits (where the integrand goes rapidly to zero anyway) make no difference.

We are left with the result that

$$\widetilde{f}(\omega) = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-\tau^2\omega^2}{2}\right), \tag{13.7}$$

which is another Gaussian distribution, centred on zero and with a root mean square deviation $\Delta\omega = 1/\tau$. It is interesting to note, and an important property, that the Fourier transform of a Gaussian is another Gaussian. ◄

In the above example the root mean square deviation in t was τ, and so it is seen that the deviations or 'spreads' in t and in ω are inversely related:

$$\Delta\omega\, \Delta t = 1,$$

independently of the value of τ. In physical terms, the narrower in time is, say, an electrical impulse the greater the spread of frequency components it must contain. Similar physical statements are valid for other pairs of Fourier-related variables, such as spatial position and wave number. In an obvious notation, $\Delta k \Delta x = 1$ for a Gaussian wave packet.

The uncertainty relations as usually expressed in quantum mechanics can be related to this if the de Broglie and Einstein relationships for momentum and energy are introduced; they are

$$p = \hbar k \qquad \text{and} \qquad E = \hbar\omega.$$

Here $\hbar$ is Planck's constant h divided by 2π. In a quantum mechanics setting $f(t)$

is a wavefunction and the distribution of the wave intensity in time is given by $|f|^2$ (also a Gaussian). Similarly, the intensity distribution in frequency is given by $|\widetilde{f}|^2$. These two distributions have respective root mean square deviations of $\tau/\sqrt{2}$ and $1/(\sqrt{2}\tau)$, giving, after incorporation of the above relations,

$$\Delta E\,\Delta t = \hbar/2 \qquad \text{and} \qquad \Delta p\,\Delta x = \hbar/2.$$

The factors of 1/2 that appear are specific to the Gaussian form, but any distribution $f(t)$ produces for the product $\Delta E \Delta t$ a quantity $\lambda\hbar$ in which λ is strictly positive (in fact, the Gaussian value of 1/2 is the minimum possible).

13.1.2 Fraunhofer diffraction

We take our final example of the Fourier transform from the field of optics. The pattern of transmitted light produced by a partially opaque (or phase-changing) object upon which a coherent beam of radiation falls is called a *diffraction pattern* and, in particular, when the cross-section of the object is small compared with the distance at which the light is observed the pattern is known as a *Fraunhofer* diffraction pattern.

We will consider only the case in which the light is monochromatic with wavelength λ. The direction of the incident beam of light can then be described by the *wave vector* $\mathbf{k}$; the magnitude of this vector is given by the *wave number* $k = 2\pi/\lambda$ of the light. The essential quantity in a Fraunhofer diffraction pattern is the dependence of the observed amplitude (and hence intensity) on the angle θ between the viewing direction $\mathbf{k}'$ and the direction $\mathbf{k}$ of the incident beam. This is entirely determined by the spatial distribution of the amplitude and phase of the light at the object, the transmitted intensity in a particular direction $\mathbf{k}'$ being determined by the corresponding Fourier component of this spatial distribution.

As an example, we take as an object a simple two-dimensional screen of width $2Y$ on which light of wave number k is incident normally; see figure 13.2. We suppose that at the position $(0, y)$ the amplitude of the transmitted light is $f(y)$ per unit length in the y-direction ($f(y)$ may be complex). The function $f(y)$ is called an *aperture function*. Both the screen and beam are assumed infinite in the z-direction.

Denoting the unit vectors in the x- and y- directions by $\mathbf{i}$ and $\mathbf{j}$ respectively, the total light amplitude at a position $\mathbf{r}_0 = x_0\mathbf{i} + y_0\mathbf{j}$, with $x_0 > 0$, will be the superposition of all the (Huyghens') wavelets originating from the various parts of the screen. For large r_0 $(= |\mathbf{r}_0|)$, these can be treated as plane waves to give[§]

$$A(\mathbf{r}_0) = \int_{-Y}^{Y} \frac{f(y)\exp[i\mathbf{k}'\cdot(\mathbf{r}_0 - y\mathbf{j})]}{|\mathbf{r}_0 - y\mathbf{j}|}\,dy. \qquad (13.8)$$

[§] This is the approach first used by Fresnel. For simplicity we have omitted from the integral a multiplicative inclination factor that depends on angle θ and decreases as θ increases.

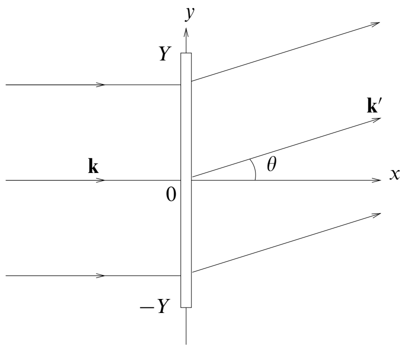

Figure 13.2 Diffraction grating of width $2Y$ with light of wavelength $2\pi/k$ being diffracted through an angle θ.

The factor $\exp[i\mathbf{k}' \cdot (\mathbf{r}_0 - y\mathbf{j})]$ represents the phase change undergone by the light in travelling from the point $y\mathbf{j}$ on the screen to the point $\mathbf{r}_0$, and the denominator represents the reduction in amplitude with distance. (Recall that the system is infinite in the z-direction and so the 'spreading' is effectively in two dimensions only.)

If the medium is the same on both sides of the screen then $\mathbf{k}' = k\cos\theta\,\mathbf{i} + k\sin\theta\,\mathbf{j}$, and if $r_0 \gg Y$ then expression (13.8) can be approximated by

$$A(\mathbf{r}_0) = \frac{\exp(i\mathbf{k}' \cdot \mathbf{r}_0)}{r_0} \int_{-\infty}^{\infty} f(y) \exp(-iky\sin\theta)\, dy. \tag{13.9}$$

We have used that $f(y) = 0$ for $|y| > Y$ to extend the integral to infinite limits. The intensity in the direction θ is then given by

$$I(\theta) = |A|^2 = \frac{2\pi}{{r_0}^2} |\widetilde{f}(q)|^2, \tag{13.10}$$

where $q = k\sin\theta$.

►*Evaluate $I(\theta)$ for an aperture consisting of two long slits each of width $2b$ whose centres are separated by a distance $2a$, $a > b$; the slits are illuminated by light of wavelength λ.*

The aperture function is plotted in figure 13.3. We first need to find $\widetilde{f}(q)$:

$$\begin{aligned}
\widetilde{f}(q) &= \frac{1}{\sqrt{2\pi}} \int_{-a-b}^{-a+b} e^{-iqx}\, dx + \frac{1}{\sqrt{2\pi}} \int_{a-b}^{a+b} e^{-iqx}\, dx \\
&= \frac{1}{\sqrt{2\pi}} \left[-\frac{e^{-iqx}}{iq} \right]_{-a-b}^{-a+b} + \frac{1}{\sqrt{2\pi}} \left[-\frac{e^{-iqx}}{iq} \right]_{a-b}^{a+b} \\
&= \frac{-1}{iq\sqrt{2\pi}} \left[e^{-iq(-a+b)} - e^{-iq(-a-b)} + e^{-iq(a+b)} - e^{-iq(a-b)} \right].
\end{aligned}$$

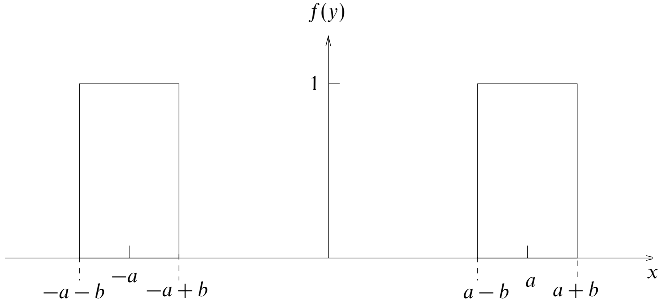

Figure 13.3 The aperture function $f(y)$ for two wide slits.

After some manipulation we obtain

$$\tilde{f}(q) = \frac{4\cos qa \sin qb}{q\sqrt{2\pi}}.$$

Now applying (13.10), and remembering that $q = (2\pi \sin\theta)/\lambda$, we find

$$I(\theta) = \frac{16\cos^2 qa \sin^2 qb}{q^2 {r_0}^2},$$

where r_0 is the distance from the centre of the aperture. ◀

13.1.3 The Dirac δ-function

Before going on to consider further properties of Fourier transforms we make a digression to discuss the Dirac δ-function and its relation to Fourier transforms. The δ-function is different from most functions encountered in the physical sciences but we will see that a rigorous mathematical definition exists; the utility of the δ-function will be demonstrated throughout the remainder of this chapter. It can be visualised as a very sharp narrow pulse (in space, time, density, etc.) which produces an integrated effect having a definite magnitude. The formal properties of the δ-function may be summarised as follows.

The Dirac δ-function has the property that

$$\delta(t) = 0 \qquad \text{for } t \neq 0, \tag{13.11}$$

but its fundamental defining property is

$$\int f(t)\delta(t-a)\,dt = f(a), \tag{13.12}$$

provided the range of integration includes the point $t = a$; otherwise the integral equals zero. This leads immediately to two further useful results:

$$\int_{-a}^{b} \delta(t)\, dt = 1 \qquad \text{for all } a, b > 0 \tag{13.13}$$

and

$$\int \delta(t-a)\, dt = 1, \tag{13.14}$$

provided the range of integration includes $t = a$.

Equation (13.12) can be used to derive further useful properties of the Dirac δ-function:

$$\delta(t) = \delta(-t), \tag{13.15}$$

$$\delta(at) = \frac{1}{|a|}\delta(t), \tag{13.16}$$

$$t\delta(t) = 0. \tag{13.17}$$

►*Prove that* $\delta(bt) = \delta(t)/|b|$.

Let us first consider the case where $b > 0$. It follows that

$$\int_{-\infty}^{\infty} f(t)\delta(bt)\, dt = \int_{-\infty}^{\infty} f\left(\frac{t'}{b}\right)\delta(t')\frac{dt'}{b} = \frac{1}{b}f(0) = \frac{1}{b}\int_{-\infty}^{\infty} f(t)\delta(t)\, dt,$$

where we have made the substitution $t' = bt$. But $f(t)$ is arbitrary and so we immediately see that $\delta(bt) = \delta(t)/b = \delta(t)/|b|$ for $b > 0$.

Now consider the case where $b = -c < 0$. It follows that

$$\begin{aligned}\int_{-\infty}^{\infty} f(t)\delta(bt)\, dt &= \int_{\infty}^{-\infty} f\left(\frac{t'}{-c}\right)\delta(t')\left(\frac{dt'}{-c}\right) = \int_{-\infty}^{\infty} \frac{1}{c}f\left(\frac{t'}{-c}\right)\delta(t')\, dt'\\ &= \frac{1}{c}f(0) = \frac{1}{|b|}f(0) = \frac{1}{|b|}\int_{-\infty}^{\infty} f(t)\delta(t)\, dt,\end{aligned}$$

where we have made the substitution $t' = bt = -ct$. But $f(t)$ is arbitrary and so

$$\delta(bt) = \frac{1}{|b|}\delta(t),$$

for all b, which establishes the result. ◄

Furthermore, by considering an integral of the form

$$\int f(t)\delta(h(t))\, dt,$$

and making a change of variables to $z = h(t)$, we may show that

$$\delta(h(t)) = \sum_i \frac{\delta(t - t_i)}{|h'(t_i)|}, \tag{13.18}$$

where the t_i are those values of t for which $h(t) = 0$ and $h'(t)$ stands for dh/dt.

The derivative of the delta function, $\delta'(t)$, is defined by

$$\int_{-\infty}^{\infty} f(t)\delta'(t)\,dt = \Big[f(t)\delta(t)\Big]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f'(t)\delta(t)\,dt$$
$$= -f'(0), \qquad (13.19)$$

and similarly for higher derivatives.

For many practical purposes, effects that are not strictly described by a δ-function may be analysed as such, if they take place in an interval much shorter than the response interval of the system on which they act. For example, the idealised notion of an impulse of magnitude J applied at time t_0 can be represented by

$$j(t) = J\delta(t - t_0). \qquad (13.20)$$

Many physical situations are described by a δ-function in space rather than in time. Moreover, we often require the δ-function to be defined in more than one dimension. For example, the charge density of a point charge q at a point $\mathbf{r}_0$ may be expressed as a three-dimensional δ-function

$$\rho(\mathbf{r}) = q\delta(\mathbf{r} - \mathbf{r_0}) = q\delta(x - x_0)\delta(y - y_0)\delta(z - z_0), \qquad (13.21)$$

so that a discrete 'quantum' is expressed as if it were a continuous distribution. From (13.21) we see that (as expected) the total charge enclosed in a volume V is given by

$$\int_V \rho(\mathbf{r})\,dV = \int_V q\delta(\mathbf{r} - \mathbf{r}_0)\,dV = \begin{cases} q & \text{if } \mathbf{r}_0 \text{ lies in } V, \\ 0 & \text{otherwise.} \end{cases}$$

Closely related to the Dirac δ-function is the *Heaviside* or *unit step function* $H(t)$, for which

$$H(t) = \begin{cases} 1 & \text{for } t > 0, \\ 0 & \text{for } t < 0. \end{cases} \qquad (13.22)$$

This function is clearly discontinuous at $t = 0$ and it is usual to take $H(0) = 1/2$. The Heaviside function is related to the delta function by

$$H'(t) = \delta(t). \qquad (13.23)$$

►*Prove relation (13.23).*

Considering the integral

$$\begin{aligned}\int_{-\infty}^{\infty} f(t)H'(t)\,dt &= \Big[f(t)H(t)\Big]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f'(t)H(t)\,dt \\ &= f(\infty) - \int_{0}^{\infty} f'(t)\,dt \\ &= f(\infty) - \Big[f(t)\Big]_{0}^{\infty} = f(0),\end{aligned}$$

and comparing it with (13.12) when $a = 0$ immediately shows that $H'(t) = \delta(t)$. ◄

13.1.4 Relation of the δ-function to Fourier transforms

In the previous section we introduced the Dirac δ-function as a way of representing very sharp narrow pulses, but in no way related it to Fourier transforms. We now show that the δ-function can equally well be defined in a way that more naturally relates it to the Fourier transform.

Referring back to the Fourier inversion theorem (13.4), we have

$$\begin{aligned}f(t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{i\omega t}\int_{-\infty}^{\infty} du\, f(u)\, e^{-i\omega u} \\ &= \int_{-\infty}^{\infty} du\ f(u)\left\{\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega(t-u)}\,d\omega\right\}.\end{aligned}$$

Comparison of this with (13.12) shows that we may write the δ-function as

$$\delta(t-u) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega(t-u)}\,d\omega. \tag{13.24}$$

Considered as a Fourier transform, this representation shows that a very narrow time peak at $t = u$ results from the superposition of a complete spectrum of harmonic waves, all frequencies having the same amplitude and all waves being in phase at $t = u$. This suggests that the δ-function may also be represented as the limit of the transform of a uniform distribution of unit height as the width of this distribution becomes infinite.

Consider the rectangular distribution of frequencies shown in figure 13.4(a). From (13.6), taking the inverse Fourier transform,

$$\begin{aligned}f_\Omega(t) &= \frac{1}{\sqrt{2\pi}}\int_{-\Omega}^{\Omega} 1\times e^{i\omega t}\,d\omega \\ &= \frac{2\Omega}{\sqrt{2\pi}}\frac{\sin\Omega t}{\Omega t}.\end{aligned} \tag{13.25}$$

This function is illustrated in figure 13.4(b) and it is apparent that, for large Ω, it becomes very large at $t = 0$ and also very narrow about $t = 0$, as we qualitatively

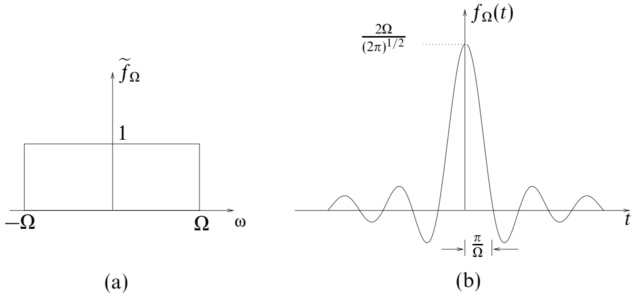

Figure 13.4 (a) A Fourier transform showing a rectangular distribution of frequencies between $\pm\Omega$; (b) the function of which it is the transform, which is proportional to $t^{-1}\sin\Omega t$.

expect and require. We also note that, in the limit $\Omega \to \infty$, $f_\Omega(t)$, as defined by the inverse Fourier transform, tends to $(2\pi)^{1/2}\delta(t)$ by virtue of (13.24). Hence we may conclude that the δ-function can also be represented by

$$\delta(t) = \lim_{\Omega\to\infty}\left(\frac{\sin\Omega t}{\pi t}\right). \tag{13.26}$$

Several other function representations are equally valid, e.g. the limiting cases of rectangular, triangular or Gaussian distributions; the only essential requirements are a knowledge of the area under such a curve and that undefined operations such as dividing by zero are not inadvertently carried out on the δ-function whilst some non-explicit representation is being employed.

We also note that the Fourier transform definition of the delta function, (13.24), shows that the latter is real since

$$\delta^*(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega t}\,d\omega = \delta(-t) = \delta(t).$$

Finally, the Fourier transform of a δ-function is simply

$$\widetilde{\delta}(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\delta(t)\,e^{-i\omega t}\,dt = \frac{1}{\sqrt{2\pi}}. \tag{13.27}$$

13.1.5 Properties of Fourier transforms

Having considered the Dirac δ-function, we now return to our discussion of the properties of Fourier transforms. As we would expect, Fourier transforms have many properties analogous to those of Fourier series in respect of the connection between the transforms of related functions. Here we list these properties without proof; they can be verified by working from the definition of the transform. As previously, we denote the Fourier transform of $f(t)$ by $\widetilde{f}(\omega)$ or $\mathscr{F}[f(t)]$.

(i) Differentiation:

$$\mathscr{F}\left[f'(t)\right] = i\omega\widetilde{f}(\omega). \tag{13.28}$$

This may be extended to higher derivatives, so that

$$\mathscr{F}\left[f''(t)\right] = i\omega\mathscr{F}\left[f'(t)\right] = -\omega^2\widetilde{f}(\omega),$$

and so on.

(ii) Integration:

$$\mathscr{F}\left[\int^t f(s)\,ds\right] = \frac{1}{i\omega}\widetilde{f}(\omega) + 2\pi c\delta(\omega), \tag{13.29}$$

where the term $2\pi c\delta(\omega)$ represents the Fourier transform of the constant of integration associated with the indefinite integral.

(iii) Scaling:

$$\mathscr{F}[f(at)] = \frac{1}{a}\widetilde{f}\left(\frac{\omega}{a}\right). \tag{13.30}$$

(iv) Translation:

$$\mathscr{F}[f(t+a)] = e^{ia\omega}\widetilde{f}(\omega). \tag{13.31}$$

(v) Exponential multiplication:

$$\mathscr{F}\left[e^{\alpha t}f(t)\right] = \widetilde{f}(\omega + i\alpha), \tag{13.32}$$

where α may be real, imaginary or complex.

►*Prove relation (13.28).*

Calculating the Fourier transform of $f'(t)$ directly, we obtain

$$\begin{aligned}\mathscr{F}\left[f'(t)\right] &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f'(t)\,e^{-i\omega t}\,dt \\ &= \frac{1}{\sqrt{2\pi}}\left[e^{-i\omega t}f(t)\right]_{-\infty}^{\infty} + \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} i\omega\,e^{-i\omega t}f(t)\,dt \\ &= i\omega\widetilde{f}(\omega),\end{aligned}$$

if $f(t) \to 0$ at $t = \pm\infty$, as it must since $\int_{-\infty}^{\infty}|f(t)|\,dt$ is finite. ◄

To illustrate a use and also a proof of (13.32), let us consider an amplitude-modulated radio wave. Suppose a message to be broadcast is represented by $f(t)$. The message can be added electronically to a constant signal a of magnitude such that $a + f(t)$ is never negative, and then the sum can be used to modulate the amplitude of a carrier signal of frequency ω_c. Using a complex exponential notation, the transmitted amplitude is now

$$g(t) = A\,[a + f(t)]\;e^{i\omega_c t}. \tag{13.33}$$

Ignoring in the present context the effect of the term $Aa\exp(i\omega_{\rm c}t)$, which gives a contribution to the transmitted spectrum only at $\omega = \omega_{\rm c}$, we obtain for the new spectrum

$$\begin{aligned}
\widetilde{g}(\omega) &= \frac{1}{\sqrt{2\pi}}A\int_{-\infty}^{\infty} f(t)\, e^{i\omega_{\rm c}t}\, e^{-i\omega t}\, dt \\
&= \frac{1}{\sqrt{2\pi}}A\int_{-\infty}^{\infty} f(t)\, e^{-i(\omega-\omega_{\rm c})t}\, dt \\
&= A\widetilde{f}(\omega-\omega_{\rm c}),
\end{aligned} \tag{13.34}$$

which is simply a shift of the whole spectrum by the carrier frequency. The use of different carrier frequencies enables signals to be separated.

13.1.6 Odd and even functions

If $f(t)$ is odd or even then we may derive alternative forms of Fourier's inversion theorem, which lead to the definition of different transform pairs. Let us first consider an odd function $f(t) = -f(-t)$, whose Fourier transform is given by

$$\begin{aligned}
\widetilde{f}(\omega) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)\, e^{-i\omega t}\, dt \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)(\cos\omega t - i\sin\omega t)\, dt \\
&= \frac{-2i}{\sqrt{2\pi}}\int_{0}^{\infty} f(t)\sin\omega t\, dt,
\end{aligned}$$

where in the last line we use the fact that $f(t)$ and $\sin\omega t$ are odd, whereas $\cos\omega t$ is even.

We note that $\widetilde{f}(-\omega) = -\widetilde{f}(\omega)$, i.e. $\widetilde{f}(\omega)$ is an odd function of ω. Hence

$$\begin{aligned}
f(t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \widetilde{f}(\omega)\, e^{i\omega t}\, d\omega = \frac{2i}{\sqrt{2\pi}}\int_{0}^{\infty} \widetilde{f}(\omega)\sin\omega t\, d\omega \\
&= \frac{2}{\pi}\int_{0}^{\infty} d\omega\, \sin\omega t\left\{\int_{0}^{\infty} f(u)\sin\omega u\, du\right\}.
\end{aligned}$$

Thus we may define the *Fourier sine transform pair* for odd functions:

$$\widetilde{f}_s(\omega) = \sqrt{\frac{2}{\pi}}\int_{0}^{\infty} f(t)\ \sin\omega t\, dt, \tag{13.35}$$

$$f(t) = \sqrt{\frac{2}{\pi}}\int_{0}^{\infty} \widetilde{f}_s(\omega)\ \sin\omega t\, d\omega. \tag{13.36}$$

Note that although the Fourier sine transform pair was derived by considering an odd function $f(t)$ defined over all t, the definitions (13.35) and (13.36) only require $f(t)$ and $\widetilde{f}_s(\omega)$ to be defined for positive t and ω respectively. For an

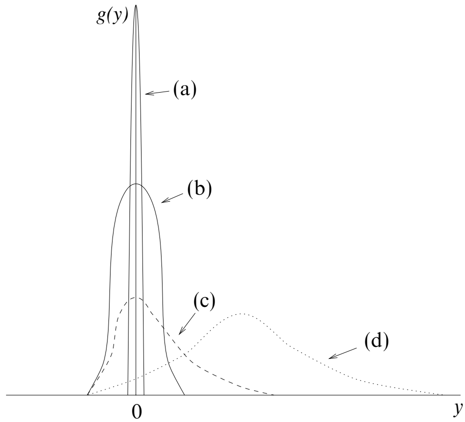

Figure 13.5 Resolution functions: (a) ideal δ-function; (b) typical unbiased resolution; (c) and (d) biases tending to shift observations to higher values than the true one.

even function, i.e. one for which $f(t) = f(-t)$, we can define the *Fourier cosine transform pair* in a similar way, but with $\sin \omega t$ replaced by $\cos \omega t$.

13.1.7 Convolution and deconvolution

It is apparent that any attempt to measure the value of a physical quantity is limited, to some extent, by the finite resolution of the measuring apparatus used. On the one hand, the physical quantity we wish to measure will be in general a function of an independent variable, x say, i.e. the true function to be measured takes the form $f(x)$. On the other hand, the apparatus we are using does not give the true output value of the function; a resolution function $g(y)$ is involved. By this we mean that the probability that an output value $y = 0$ will be recorded instead as being between y and $y+dy$ is given by $g(y)\,dy$. Some possible resolution functions of this sort are shown in figure 13.5. To obtain good results we wish the resolution function to be as close to a δ-function as possible (case (*a*)). A typical piece of apparatus has a resolution function of finite width, although if it is accurate the mean is centred on the true value (case (*b*)). However, some apparatus may show a bias that tends to shift observations to higher or lower values than the true ones (cases (*c*) and (*d*)), thereby exhibiting systematic error.

Given that the true distribution is $f(x)$ and the resolution function of our measuring apparatus is $g(y)$, we wish to calculate what the observed distribution $h(z)$ will be. The symbols x, y and z all refer to the same physical variable (e.g.

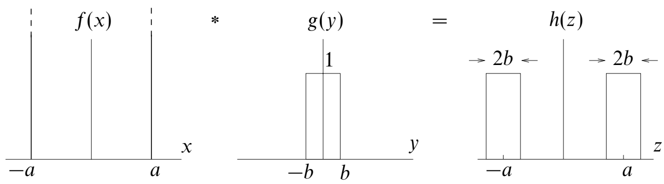

Figure 13.6 The convolution of two functions $f(x)$ and $g(y)$.

length or angle), but are denoted differently because the variable appears in the analysis in three different roles.

The probability that a true reading lying between x and $x + dx$, and so having probability $f(x)\,dx$ of being selected by the experiment, will be moved by the instrumental resolution by an amount $z - x$ into a small interval of width dz is $g(z - x)\,dz$. Hence the combined probability that the interval dx will give rise to an observation appearing in the interval dz is $f(x)\,dx\,g(z-x)\,dz$. Adding together the contributions from all values of x that can lead to an observation in the range z to $z + dz$, we find that the observed distribution is given by

$$h(z) = \int_{-\infty}^{\infty} f(x)g(z - x)\,dx. \tag{13.37}$$

The integral in (13.37) is called the *convolution* of the functions f and g and is often written $f * g$. The convolution defined above is commutative ($f * g = g * f$), associative and distributive. The observed distribution is thus the convolution of the true distribution and the experimental resolution function. The result will be that the observed distribution is broader and smoother than the true one and, if $g(y)$ has a bias, the maxima will normally be displaced from their true positions. It is also obvious from (13.37) that if the resolution is the ideal δ-function, $g(y) = \delta(y)$ then $h(z) = f(z)$ and the observed distribution is the true one.

It is interesting to note, and a very important property, that the convolution of any function $g(y)$ with a number of delta functions leaves a copy of $g(y)$ at the position of each of the delta functions.

►*Find the convolution of the function $f(x) = \delta(x + a) + \delta(x - a)$ with the function $g(y)$ plotted in figure 13.6.*

Using the convolution integral (13.37)

$$h(z) = \int_{-\infty}^{\infty} f(x)g(z - x)\,dx = \int_{-\infty}^{\infty} [\delta(x + a) + \delta(x - a)]g(z - x)\,dx$$
$$= g(z + a) + g(z - a).$$

This convolution $h(z)$ is plotted in figure 13.6. ◄

Let us now consider the Fourier transform of the convolution (13.37); this is given by

$$\begin{aligned}\widetilde{h}(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dz\, e^{-ikz}\left\{\int_{-\infty}^{\infty} f(x)g(z-x)\,dx\right\}\\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, f(x)\left\{\int_{-\infty}^{\infty} g(z-x)\,e^{-ikz}\,dz\right\}.\end{aligned}$$

If we let $u = z - x$ in the second integral we have

$$\begin{aligned}\widetilde{h}(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, f(x)\left\{\int_{-\infty}^{\infty} g(u)\,e^{-ik(u+x)}\,du\right\}\\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)\,e^{-ikx}\,dx\int_{-\infty}^{\infty} g(u)\,e^{-iku}\,du\\ &= \frac{1}{\sqrt{2\pi}}\times\sqrt{2\pi}\,\widetilde{f}(k)\times\sqrt{2\pi}\,\widetilde{g}(k) = \sqrt{2\pi}\,\widetilde{f}(k)\widetilde{g}(k). \qquad (13.38)\end{aligned}$$

Hence the Fourier transform of a convolution $f * g$ is equal to the product of the separate Fourier transforms multiplied by $\sqrt{2\pi}$; this result is called the *convolution theorem*.

It may be proved similarly that the converse is also true, namely that the Fourier transform of the product $f(x)g(x)$ is given by

$$\mathscr{F}[f(x)g(x)] = \frac{1}{\sqrt{2\pi}}\widetilde{f}(k) * \widetilde{g}(k). \qquad (13.39)$$

►*Find the Fourier transform of the function in figure 13.3 representing two wide slits by considering the Fourier transforms of* (i) *two δ-functions, at $x = \pm a$,* (ii) *a rectangular function of height* 1 *and width* $2b$ *centred on* $x = 0$.

(i) The Fourier transform of the two δ-functions is given by

$$\begin{aligned}\widetilde{f}(q) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\delta(x-a)\,e^{-iqx}\,dx + \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\delta(x+a)\,e^{-iqx}\,dx\\ &= \frac{1}{\sqrt{2\pi}}\left(e^{-iqa}+e^{iqa}\right) = \frac{2\cos qa}{\sqrt{2\pi}}.\end{aligned}$$

(ii) The Fourier transform of the broad slit is

$$\begin{aligned}\widetilde{g}(q) &= \frac{1}{\sqrt{2\pi}}\int_{-b}^{b} e^{-iqx}\,dx = \frac{1}{\sqrt{2\pi}}\left[\frac{e^{-iqx}}{-iq}\right]_{-b}^{b}\\ &= \frac{-1}{iq\sqrt{2\pi}}(e^{-iqb}-e^{iqb}) = \frac{2\sin qb}{q\sqrt{2\pi}}.\end{aligned}$$

We have already seen that the convolution of these functions is the required function representing two wide slits (see figure 13.6). So, using the convolution theorem, the Fourier transform of the convolution is $\sqrt{2\pi}$ times the product of the individual transforms, i.e. $4\cos qa\,\sin qb/(q\sqrt{2\pi})$. This is, of course, the same result as that obtained in the example in subsection 13.1.2. ◄

The inverse of convolution, called *deconvolution*, allows us to find a true distribution $f(x)$ given an observed distribution $h(z)$ and a resolution function $g(y)$.

►*An experimental quantity $f(x)$ is measured using apparatus with a known resolution function $g(y)$ to give an observed distribution $h(z)$. How may $f(x)$ be extracted from the measured distribution?*

From the convolution theorem (13.38), the Fourier transform of the measured distribution is

$$\widetilde{h}(k) = \sqrt{2\pi}\,\widetilde{f}(k)\widetilde{g}(k),$$

from which we obtain

$$\widetilde{f}(k) = \frac{1}{\sqrt{2\pi}}\frac{\widetilde{h}(k)}{\widetilde{g}(k)}.$$

Then on inverse Fourier transforming we find

$$f(x) = \frac{1}{\sqrt{2\pi}}\mathscr{F}^{-1}\left[\frac{\widetilde{h}(k)}{\widetilde{g}(k)}\right].$$

In words, to extract the true distribution, we divide the Fourier transform of the observed distribution by that of the resolution function for each value of k and then take the inverse Fourier transform of the function so generated. ◄

This explicit method of extracting true distributions is straightforward for exact functions but, in practice, because of experimental and statistical uncertainties in the experimental data or because data over only a limited range are available, it is often not very precise, involving as it does three (numerical) transforms each requiring in principle an integral over an infinite range.

13.1.8 Correlation functions and energy spectra

The *cross-correlation* of two functions f and g is defined by

$$C(z) = \int_{-\infty}^{\infty} f^*(x)g(x+z)\,dx. \qquad (13.40)$$

Despite the formal similarity between (13.40) and the definition of the convolution in (13.37), the use and interpretation of the cross-correlation and of the convolution are very different; the cross-correlation provides a quantitative measure of the similarity of two functions f and g as one is displaced through a distance z relative to the other. The cross-correlation is often notated as $C = f \otimes g$, and, like convolution, it is both associative and distributive. Unlike convolution, however, it is *not* commutative, in fact

$$[f \otimes g](z) = [g \otimes f]^*(-z). \qquad (13.41)$$

►*Prove the Wiener–Kinchin theorem,*

$$\tilde{C}(k) = \sqrt{2\pi}\,[\tilde{f}(k)]^*\tilde{g}(k). \tag{13.42}$$

Following a method similar to that for the convolution of f and g, let us consider the Fourier transform of (13.40):

$$\begin{aligned}\tilde{C}(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dz\, e^{-ikz}\left\{\int_{-\infty}^{\infty} f^*(x)g(x+z)\,dx\right\}\\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, f^*(x)\left\{\int_{-\infty}^{\infty} g(x+z)\,e^{-ikz}\,dz\right\}.\end{aligned}$$

Making the substitution $u = x + z$ in the second integral we obtain

$$\begin{aligned}\tilde{C}(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, f^*(x)\left\{\int_{-\infty}^{\infty} g(u)\,e^{-ik(u-x)}\,du\right\}\\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f^*(x)\,e^{ikx}\,dx\int_{-\infty}^{\infty} g(u)\,e^{-iku}\,du\\ &= \frac{1}{\sqrt{2\pi}}\times\sqrt{2\pi}\,[\tilde{f}(k)]^*\times\sqrt{2\pi}\,\tilde{g}(k) = \sqrt{2\pi}\,[\tilde{f}(k)]^*\tilde{g}(k). \blacktriangleleft\end{aligned}$$

Thus the Fourier transform of the cross-correlation of f and g is equal to the product of $[\tilde{f}(k)]^*$ and $\tilde{g}(k)$ multiplied by $\sqrt{2\pi}$. This a statement of the *Wiener–Kinchin theorem.* Similarly we can derive the converse theorem

$$\mathcal{F}\left[f^*(x)g(x)\right] = \frac{1}{\sqrt{2\pi}}\tilde{f}\otimes\tilde{g}.$$

If we now consider the special case where g is taken to be equal to f in (13.40) then, writing the LHS as $a(z)$, we have

$$a(z) = \int_{-\infty}^{\infty} f^*(x)f(x+z)\,dx; \tag{13.43}$$

this is called the *auto-correlation function* of $f(x)$. Using the Wiener–Kinchin theorem (13.42) we see that

$$\begin{aligned}a(z) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \tilde{a}(k)\,e^{ikz}\,dk\\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \sqrt{2\pi}\,[\tilde{f}(k)]^*\tilde{f}(k)\,e^{ikz}\,dk,\end{aligned}$$

so that $a(z)$ is the inverse Fourier transform of $\sqrt{2\pi}\,|\tilde{f}(k)|^2$, which is in turn called the *energy spectrum* of f.

13.1.9 Parseval's theorem

Using the results of the previous section we can immediately obtain *Parseval's theorem.* The most general form of this (also called the *multiplication theorem*) is obtained simply by noting from (13.42) that the cross-correlation (13.40) of two functions f and g can be written as

$$C(z) = \int_{-\infty}^{\infty} f^*(x)g(x+z)\,dx = \int_{-\infty}^{\infty} [\widetilde{f}(k)]^*\widetilde{g}(k)\,e^{ikz}\,dk. \tag{13.44}$$

Then, setting $z = 0$ gives the multiplication theorem

$$\int_{-\infty}^{\infty} f^*(x)g(x)\,dx = \int [\widetilde{f}(k)]^*\widetilde{g}(k)\,dk. \tag{13.45}$$

Specialising further, by letting $g = f$, we derive the most common form of Parseval's theorem,

$$\int_{-\infty}^{\infty} |f(x)|^2\,dx = \int_{-\infty}^{\infty} |\widetilde{f}(k)|^2\,dk. \tag{13.46}$$

When f is a physical amplitude these integrals relate to the total intensity involved in some physical process. We have already met a form of Parseval's theorem for Fourier series in chapter 12; it is in fact a special case of (13.46).

►*The displacement of a damped harmonic oscillator as a function of time is given by*

$$f(t) = \begin{cases} 0 & \text{for } t < 0, \\ e^{-t/\tau}\sin\omega_0 t & \text{for } t \geq 0. \end{cases}$$

Find the Fourier transform of this function and so give a physical interpretation of Parseval's theorem.

Using the usual definition for the Fourier transform we find

$$\widetilde{f}(\omega) = \int_{-\infty}^{0} 0 \times e^{-i\omega t}\,dt + \int_{0}^{\infty} e^{-t/\tau}\sin\omega_0 t\,e^{-i\omega t}\,dt.$$

Writing $\sin\omega_0 t$ as $(e^{i\omega_0 t} - e^{-i\omega_0 t})/2i$ we obtain

$$\begin{aligned}\widetilde{f}(\omega) &= 0 + \frac{1}{2i}\int_0^{\infty} \left[e^{-it(\omega-\omega_0-i/\tau)} - e^{-it(\omega+\omega_0-i/\tau)}\right] dt \\ &= \frac{1}{2}\left[\frac{1}{\omega+\omega_0-i/\tau} - \frac{1}{\omega-\omega_0-i/\tau}\right],\end{aligned}$$

which is the required Fourier transform. The physical interpretation of $|\widetilde{f}(\omega)|^2$ is the energy content per unit frequency interval (i.e. the *energy spectrum*) whilst $|f(t)|^2$ is proportional to the sum of the kinetic and potential energies of the oscillator. Hence (to within a constant) Parseval's theorem shows the equivalence of these two alternative specifications for the total energy. ◄

13.1.10 Fourier transforms in higher dimensions

The concept of the Fourier transform can be extended naturally to more than one dimension. For instance we may wish to find the spatial Fourier transform of two- or three-dimensional functions of position. For example, in three dimensions we can define the Fourier transform of $f(x, y, z)$ as

$$\widetilde{f}(k_x, k_y, k_z) = \frac{1}{(2\pi)^{3/2}} \iiint f(x, y, z)\, e^{-ik_x x} e^{-ik_y y} e^{-ik_z z}\, dx\, dy\, dz, \tag{13.47}$$

and its inverse as

$$f(x, y, z) = \frac{1}{(2\pi)^{3/2}} \iiint \widetilde{f}(k_x, k_y, k_z)\, e^{ik_x x} e^{ik_y y} e^{ik_z z}\, dk_x\, dk_y\, dk_z. \tag{13.48}$$

Denoting the vector with components k_x, k_y, k_z by $\mathbf{k}$ and that with components x, y, z by $\mathbf{r}$, we can write the Fourier transform pair (13.47), (13.48) as

$$\widetilde{f}(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int f(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{r}}\, d^3\mathbf{r}, \tag{13.49}$$

$$f(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int \widetilde{f}(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{r}}\, d^3\mathbf{k}. \tag{13.50}$$

From these relations we may deduce that the three-dimensional Dirac δ-function can be written as

$$\delta(\mathbf{r}) = \frac{1}{(2\pi)^3} \int e^{i\mathbf{k}\cdot\mathbf{r}}\, d^3\mathbf{k}. \tag{13.51}$$

Similar relations to (13.49), (13.50) and (13.51) exist for spaces of other dimensionalities.

►*In three-dimensional space a function $f(\mathbf{r})$ possesses spherical symmetry, so that $f(\mathbf{r}) = f(r)$. Find the Fourier transform of $f(\mathbf{r})$ as a one-dimensional integral.*

Let us choose spherical polar coordinates in which the vector $\mathbf{k}$ of the Fourier transform lies along the polar axis ($\theta = 0$). This we can do since $f(\mathbf{r})$ is spherically symmetric. We then have

$$d^3\mathbf{r} = r^2 \sin\theta\, dr\, d\theta\, d\phi \qquad \text{and} \qquad \mathbf{k}\cdot\mathbf{r} = kr\cos\theta,$$

where $k = |\mathbf{k}|$. The Fourier transform is then given by

$$\begin{aligned}
\widetilde{f}(\mathbf{k}) &= \frac{1}{(2\pi)^{3/2}} \int f(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{r}}\, d^3\mathbf{r} \\
&= \frac{1}{(2\pi)^{3/2}} \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi\, f(r) r^2 \sin\theta\, e^{-ikr\cos\theta} \\
&= \frac{1}{(2\pi)^{3/2}} \int_0^\infty dr\, 2\pi f(r) r^2 \int_0^\pi d\theta\, \sin\theta\, e^{-ikr\cos\theta}.
\end{aligned}$$

The integral over θ may be straightforwardly evaluated by noting that

$$\frac{d}{d\theta}(e^{-ikr\cos\theta}) = ikr \sin\theta\, e^{-ikr\cos\theta}.$$

Therefore

$$\begin{aligned}
\widetilde{f}(\mathbf{k}) &= \frac{1}{(2\pi)^{3/2}} \int_0^\infty dr\, 2\pi f(r) r^2 \left[\frac{e^{-ikr\cos\theta}}{ikr}\right]_{\theta=0}^{\theta=\pi} \\
&= \frac{1}{(2\pi)^{3/2}} \int_0^\infty 4\pi r^2 f(r) \left(\frac{\sin kr}{kr}\right) dr. \blacktriangleleft
\end{aligned}$$

A similar result may be obtained for two-dimensional Fourier transforms in which $f(\mathbf{r}) = f(\rho)$, i.e. $f(\mathbf{r})$ is independent of azimuthal angle ϕ. In this case, using the integral representation of the Bessel function $J_0(x)$ given at the very end of subsection 18.5.3, we find

$$\widetilde{f}(\mathbf{k}) = \frac{1}{2\pi}\int_0^\infty 2\pi\rho f(\rho)J_0(k\rho)\,d\rho. \tag{13.52}$$

13.2 Laplace transforms

Often we are interested in functions $f(t)$ for which the Fourier transform does not exist because $f \not\to 0$ as $t \to \infty$, and so the integral defining $\widetilde{f}$ does not converge. This would be the case for the function $f(t) = t$, which does not possess a Fourier transform. Furthermore, we might be interested in a given function only for $t > 0$, for example when we are given the value at $t = 0$ in an initial-value problem. This leads us to consider the Laplace transform, $\bar{f}(s)$ or $\mathscr{L}[f(t)]$, of $f(t)$, which is defined by

$$\bar{f}(s) \equiv \int_0^\infty f(t)e^{-st}\,dt, \tag{13.53}$$

provided that the integral exists. We assume here that s is real, but complex values would have to be considered in a more detailed study. In practice, for a given function $f(t)$ there will be some real number s_0 such that the integral in (13.53) exists for $s > s_0$ but diverges for $s \le s_0$.

Through (13.53) we define a *linear* transformation $\mathscr{L}$ that converts functions of the variable t to functions of a new variable s:

$$\mathscr{L}[af_1(t) + bf_2(t)] = a\mathscr{L}[f_1(t)] + b\mathscr{L}[f_2(t)] = a\bar{f}_1(s) + b\bar{f}_2(s). \tag{13.54}$$

►*Find the Laplace transforms of the functions* (i) $f(t) = 1$, (ii) $f(t) = e^{at}$, (iii) $f(t) = t^n$, *for* $n = 0, 1, 2, \ldots$.

(i) By direct application of the definition of a Laplace transform (13.53), we find

$$\mathscr{L}[1] = \int_0^\infty e^{-st}\,dt = \left[\frac{-1}{s}e^{-st}\right]_0^\infty = \frac{1}{s}, \qquad \text{if } s > 0,$$

where the restriction $s > 0$ is required for the integral to exist.

(ii) Again using (13.53) directly, we find

$$\begin{aligned}\bar{f}(s) &= \int_0^\infty e^{at}e^{-st}\,dt = \int_0^\infty e^{(a-s)t}\,dt \\ &= \left[\frac{e^{(a-s)t}}{a-s}\right]_0^\infty = \frac{1}{s-a} \qquad \text{if } s > a.\end{aligned}$$

(iii) Once again using the definition (13.53) we have

$$\bar{f}_n(s) = \int_0^\infty t^n e^{-st}\, dt.$$

Integrating by parts we find

$$\begin{aligned}\bar{f}_n(s) &= \left[\frac{-t^n e^{-st}}{s}\right]_0^\infty + \frac{n}{s}\int_0^\infty t^{n-1}e^{-st}\, dt \\ &= 0 + \frac{n}{s}\bar{f}_{n-1}(s), \qquad \text{if } s > 0.\end{aligned}$$

We now have a recursion relation between successive transforms and by calculating $\bar{f}_0$ we can infer $\bar{f}_1$, $\bar{f}_2$, etc. Since $t^0 = 1$, (i) above gives

$$\bar{f}_0 = \frac{1}{s}, \qquad \text{if } s > 0, \tag{13.55}$$

and

$$\bar{f}_1(s) = \frac{1}{s^2}, \qquad \bar{f}_2(s) = \frac{2!}{s^3}, \qquad \ldots, \qquad \bar{f}_n(s) = \frac{n!}{s^{n+1}} \qquad \text{if } s > 0.$$

Thus, in each case (i)–(iii), direct application of the definition of the Laplace transform (13.53) yields the required result. ◄

Unlike that for the Fourier transform, the inversion of the Laplace transform is not an easy operation to perform, since an explicit formula for $f(t)$, given $\bar{f}(s)$, is not straightforwardly obtained from (13.53). The general method for obtaining an inverse Laplace transform makes use of complex variable theory and is not discussed until chapter 25. However, progress can be made without having to find an *explicit* inverse, since we can prepare from (13.53) a 'dictionary' of the Laplace transforms of common functions and, when faced with an inversion to carry out, hope to find the given transform (together with its parent function) in the listing. Such a list is given in table 13.1.

When finding inverse Laplace transforms using table 13.1, it is useful to note that for all practical purposes the inverse Laplace transform is unique§ and linear so that

$$\mathscr{L}^{-1}\left[a\bar{f}_1(s) + b\bar{f}_2(s)\right] = af_1(t) + bf_2(t). \tag{13.56}$$

In many practical problems the method of partial fractions can be useful in producing an expression from which the inverse Laplace transform can be found.

►*Using table 13.1 find $f(t)$ if*

$$\bar{f}(s) = \frac{s+3}{s(s+1)}.$$

Using partial fractions $\bar{f}(s)$ may be written

$$\bar{f}(s) = \frac{3}{s} - \frac{2}{s+1}.$$

§ This is not strictly true, since two functions can differ from one another at a finite number of isolated points but have the *same* Laplace transform.

$f(t)$	$\bar{f}(s)$	s_0
c	c/s	0
ct^n	$cn!/s^{n+1}$	0
$\sin bt$	$b/(s^2+b^2)$	0
$\cos bt$	$s/(s^2+b^2)$	0
e^{at}	$1/(s-a)$	a
$t^n e^{at}$	$n!/(s-a)^{n+1}$	a
$\sinh at$	$a/(s^2-a^2)$	$\lvert a\rvert$
$\cosh at$	$s/(s^2-a^2)$	$\lvert a\rvert$
$e^{at}\sin bt$	$b/[(s-a)^2+b^2]$	a
$e^{at}\cos bt$	$(s-a)/[(s-a)^2+b^2]$	a
$t^{1/2}$	$\frac{1}{2}(\pi/s^3)^{1/2}$	0
$t^{-1/2}$	$(\pi/s)^{1/2}$	0
$\delta(t-t_0)$	e^{-st_0}	0
$H(t-t_0)=\begin{cases}1 & \text{for } t\geq t_0\\ 0 & \text{for } t<t_0\end{cases}$	e^{-st_0}/s	0

Table 13.1 Standard Laplace transforms. The transforms are valid for $s > s_0$.

Comparing this with the standard Laplace transforms in table 13.1, we find that the inverse transform of $3/s$ is 3 for $s > 0$ and the inverse transform of $2/(s+1)$ is $2e^{-t}$ for $s > -1$, and so

$$f(t) = 3 - 2e^{-t}, \qquad \text{if } s > 0. \blacktriangleleft$$

13.2.1 Laplace transforms of derivatives and integrals

One of the main uses of Laplace transforms is in solving differential equations. Differential equations are the subject of the next six chapters and we will return to the application of Laplace transforms to their solution in chapter 15. In the meantime we will derive the required results, i.e. the Laplace transforms of derivatives.

The Laplace transform of the first derivative of $f(t)$ is given by

$$\begin{aligned}\mathscr{L}\left[\frac{df}{dt}\right] &= \int_0^\infty \frac{df}{dt}e^{-st}\,dt\\ &= \left[f(t)e^{-st}\right]_0^\infty + s\int_0^\infty f(t)e^{-st}\,dt\\ &= -f(0) + s\bar{f}(s), \qquad \text{for } s > 0. \end{aligned} \tag{13.57}$$

The evaluation relies on integration by parts and higher-order derivatives may be found in a similar manner.

►*Find the Laplace transform of d^2f/dt^2.*

Using the definition of the Laplace transform and integrating by parts we obtain

$$\begin{aligned}\mathcal{L}\left[\frac{d^2f}{dt^2}\right] &= \int_0^\infty \frac{d^2f}{dt^2}e^{-st}\,dt\\ &= \left[\frac{df}{dt}e^{-st}\right]_0^\infty + s\int_0^\infty \frac{df}{dt}e^{-st}\,dt\\ &= -\frac{df}{dt}(0) + s[s\bar{f}(s) - f(0)], \qquad \text{for } s > 0,\end{aligned}$$

where (13.57) has been substituted for the integral. This can be written more neatly as

$$\mathcal{L}\left[\frac{d^2f}{dt^2}\right] = s^2\bar{f}(s) - sf(0) - \frac{df}{dt}(0), \qquad \text{for } s > 0. \blacktriangleleft$$

In general the Laplace transform of the nth derivative is given by

$$\mathcal{L}\left[\frac{d^nf}{dt^n}\right] = s^n\bar{f} - s^{n-1}f(0) - s^{n-2}\frac{df}{dt}(0) - \cdots - \frac{d^{n-1}f}{dt^{n-1}}(0), \qquad \text{for } s > 0. \tag{13.58}$$

We now turn to integration, which is much more straightforward. From the definition (13.53),

$$\begin{aligned}\mathcal{L}\left[\int_0^t f(u)\,du\right] &= \int_0^\infty dt\,e^{-st}\int_0^t f(u)\,du\\ &= \left[-\frac{1}{s}e^{-st}\int_0^t f(u)\,du\right]_0^\infty + \int_0^\infty \frac{1}{s}e^{-st}f(t)\,dt.\end{aligned}$$

The first term on the RHS vanishes at both limits, and so

$$\mathcal{L}\left[\int_0^t f(u)\,du\right] = \frac{1}{s}\mathcal{L}[f]. \tag{13.59}$$

13.2.2 Other properties of Laplace transforms

From table 13.1 it will be apparent that multiplying a function $f(t)$ by e^{at} has the effect on its transform that s is replaced by $s - a$. This is easily proved generally:

$$\begin{aligned}\mathcal{L}\left[e^{at}f(t)\right] &= \int_0^\infty f(t)e^{at}e^{-st}\,dt\\ &= \int_0^\infty f(t)e^{-(s-a)t}\,dt\\ &= \bar{f}(s-a).\end{aligned} \tag{13.60}$$

As it were, multiplying $f(t)$ by e^{at} moves the origin of s by an amount a.

We may now consider the effect of multiplying the Laplace transform $\bar{f}(s)$ by e^{-bs} $(b > 0)$. From the definition (13.53),

$$e^{-bs}\bar{f}(s) = \int_0^\infty e^{-s(t+b)} f(t)\,dt$$
$$= \int_0^\infty e^{-sz} f(z-b)\,dz,$$

on putting $t + b = z$. Thus $e^{-bs}\bar{f}(s)$ is the Laplace transform of a function $g(t)$ defined by

$$g(t) = \begin{cases} 0 & \text{for } 0 < t \le b, \\ f(t-b) & \text{for } t > b. \end{cases}$$

In other words, the function f has been translated to 'later' t (larger values of t) by an amount b.

Further properties of Laplace transforms can be proved in similar ways and are listed below.

(i) $$\mathscr{L}\left[f(at)\right] = \frac{1}{a}\bar{f}\left(\frac{s}{a}\right), \tag{13.61}$$

(ii) $$\mathscr{L}\left[t^n f(t)\right] = (-1)^n \frac{d^n \bar{f}(s)}{ds^n}, \qquad \text{for } n = 1, 2, 3, \ldots, \tag{13.62}$$

(iii) $$\mathscr{L}\left[\frac{f(t)}{t}\right] = \int_s^\infty \bar{f}(u)\,du, \tag{13.63}$$

provided $\lim_{t\to 0}[f(t)/t]$ exists.

Related results may be easily proved.

►*Find an expression for the Laplace transform of $t\,d^2f/dt^2$.*

From the definition of the Laplace transform we have

$$\mathscr{L}\left[t\frac{d^2 f}{dt^2}\right] = \int_0^\infty e^{-st}\, t\frac{d^2 f}{dt^2}\,dt$$
$$= -\frac{d}{ds}\int_0^\infty e^{-st}\frac{d^2 f}{dt^2}\,dt$$
$$= -\frac{d}{ds}[s^2\bar{f}(s) - sf(0) - f'(0)]$$
$$= -s^2\frac{d\bar{f}}{ds} - 2s\bar{f} + f(0). \blacktriangleleft$$

Finally we mention the convolution theorem for Laplace transforms (which is analogous to that for Fourier transforms discussed in subsection 13.1.7). If the functions f and g have Laplace transforms $\bar{f}(s)$ and $\bar{g}(s)$ then

$$\mathscr{L}\left[\int_0^t f(u)g(t-u)\,du\right] = \bar{f}(s)\bar{g}(s), \tag{13.64}$$

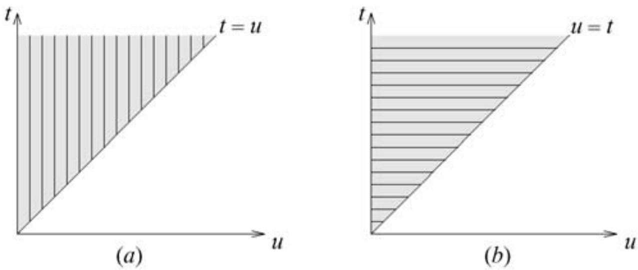

Figure 13.7 Two representations of the Laplace transform convolution (see text).

where the integral in the brackets on the LHS is the *convolution* of f and g, denoted by $f * g$. As in the case of Fourier transforms, the convolution defined above is commutative, i.e. $f * g = g * f$, and is associative and distributive. From (13.64) we also see that

$$\mathcal{L}^{-1}\left[\bar{f}(s)\bar{g}(s)\right] = \int_0^t f(u)g(t-u)\,du = f * g.$$

►*Prove the convolution theorem (13.64) for Laplace transforms.*

From the definition (13.64),

$$\begin{aligned}\bar{f}(s)\bar{g}(s) &= \int_0^\infty e^{-su} f(u)\,du \int_0^\infty e^{-sv} g(v)\,dv \\ &= \int_0^\infty du \int_0^\infty dv\, e^{-s(u+v)} f(u)g(v).\end{aligned}$$

Now letting $u + v = t$ changes the limits on the integrals, with the result that

$$\bar{f}(s)\bar{g}(s) = \int_0^\infty du\, f(u) \int_u^\infty dt\, g(t-u)\, e^{-st}.$$

As shown in figure 13.7(a) the shaded area of integration may be considered as the sum of vertical strips. However, we may instead integrate over this area by summing over horizontal strips as shown in figure 13.7(b). Then the integral can be written as

$$\begin{aligned}\bar{f}(s)\bar{g}(s) &= \int_0^t du\, f(u) \int_0^\infty dt\, g(t-u)\, e^{-st} \\ &= \int_0^\infty dt\, e^{-st} \left\{ \int_0^t f(u)g(t-u)\,du \right\} \\ &= \mathcal{L}\left[\int_0^t f(u)g(t-u)\,du\right]. \blacktriangleleft\end{aligned}$$

The properties of the Laplace transform derived in this section can sometimes be useful in finding the Laplace transforms of particular functions.

►*Find the Laplace transform of* $f(t) = t \sin bt$.

Although we could calculate the Laplace transform directly, we can use (13.62) to give

$$\bar{f}(s) = (-1)\frac{d}{ds}\mathcal{L}\,[\sin bt] = -\frac{d}{ds}\left(\frac{b}{s^2+b^2}\right) = \frac{2bs}{(s^2+b^2)^2}, \qquad \text{for } s > 0. \blacktriangleleft$$

13.3 Concluding remarks

In this chapter we have discussed Fourier and Laplace transforms in some detail. Both are examples of *integral transforms*, which can be considered in a more general context.

A general integral transform of a function $f(t)$ takes the form

$$F(\alpha) = \int_a^b K(\alpha, t) f(t)\, dt, \tag{13.65}$$

where $F(\alpha)$ is the transform of $f(t)$ with respect to the *kernel* $K(\alpha, t)$, and α is the transform variable. For example, in the Laplace transform case $K(s, t) = e^{-st}$, $a = 0$, $b = \infty$.

Very often the inverse transform can also be written straightforwardly and we obtain a transform pair similar to that encountered in Fourier transforms. Examples of such pairs are

(i) the Hankel transform

$$F(k) = \int_0^\infty f(x) J_n(kx) x\, dx,$$
$$f(x) = \int_0^\infty F(k) J_n(kx) k\, dk,$$

where the J_n are Bessel functions of order n, and

(ii) the Mellin transform

$$F(z) = \int_0^\infty t^{z-1} f(t)\, dt,$$
$$f(t) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} t^{-z} F(z)\, dz.$$

Although we do not have the space to discuss their general properties, the reader should at least be aware of this wider class of integral transforms.

13.4 Exercises

13.1 Find the Fourier transform of the function $f(t) = \exp(-|t|)$.

(a) By applying Fourier's inversion theorem prove that

$$\frac{\pi}{2}\exp(-|t|) = \int_0^\infty \frac{\cos\omega t}{1+\omega^2}\,d\omega.$$

(b) By making the substitution $\omega = \tan\theta$, demonstrate the validity of Parseval's theorem for this function.

13.2 Use the general definition and properties of Fourier transforms to show the following.

(a) If $f(x)$ is periodic with period a then $\tilde{f}(k) = 0$, unless $ka = 2\pi n$ for integer n.
(b) The Fourier transform of $tf(t)$ is $id\tilde{f}(\omega)/d\omega$.
(c) The Fourier transform of $f(mt + c)$ is

$$\frac{e^{i\omega c/m}}{m}\tilde{f}\left(\frac{\omega}{m}\right).$$

13.3 Find the Fourier transform of $H(x-a)e^{-bx}$, where $H(x)$ is the Heaviside function.

13.4 Prove that the Fourier transform of the function $f(t)$ defined in the tf-plane by straight-line segments joining $(-T, 0)$ to $(0, 1)$ to $(T, 0)$, with $f(t) = 0$ outside $|t| < T$, is

$$\tilde{f}(\omega) = \frac{T}{\sqrt{2\pi}}\operatorname{sinc}^2\left(\frac{\omega T}{2}\right),$$

where sinc x is defined as $(\sin x)/x$.

Use the general properties of Fourier transforms to determine the transforms of the following functions, graphically defined by straight-line segments and equal to zero outside the ranges specified:

(a) $(0,0)$ to $(0.5,1)$ to $(1,0)$ to $(2,2)$ to $(3,0)$ to $(4.5,3)$ to $(6,0)$;
(b) $(-2,0)$ to $(-1,2)$ to $(1,2)$ to $(2,0)$;
(c) $(0,0)$ to $(0,1)$ to $(1,2)$ to $(1,0)$ to $(2,-1)$ to $(2,0)$.

13.5 By taking the Fourier transform of the equation

$$\frac{d^2\phi}{dx^2} - K^2\phi = f(x),$$

show that its solution, $\phi(x)$, can be written as

$$\phi(x) = \frac{-1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{e^{ikx}\widetilde{f}(k)}{k^2+K^2}\,dk,$$

where $\widetilde{f}(k)$ is the Fourier transform of $f(x)$.

13.6 By differentiating the definition of the Fourier sine transform $\tilde{f}_s(\omega)$ of the function $f(t) = t^{-1/2}$ with respect to ω, and then integrating the resulting expression by parts, find an elementary differential equation satisfied by $\tilde{f}_s(\omega)$. Hence show that this function is its own Fourier sine transform, i.e. $\tilde{f}_s(\omega) = Af(\omega)$, where A is a constant. Show that it is also its own Fourier cosine transform. Assume that the limit as $x \to \infty$ of $x^{1/2}\sin\alpha x$ can be taken as zero.

13.7 Find the Fourier transform of the unit rectangular distribution

$$f(t) = \begin{cases} 1 & |t| < 1, \\ 0 & \text{otherwise.} \end{cases}$$

Determine the convolution of f with itself and, without further integration, deduce its transform. Deduce that

$$\int_{-\infty}^{\infty} \frac{\sin^2 \omega}{\omega^2}\, d\omega = \pi,$$
$$\int_{-\infty}^{\infty} \frac{\sin^4 \omega}{\omega^4}\, d\omega = \frac{2\pi}{3}.$$

13.8 Calculate the Fraunhofer spectrum produced by a diffraction grating, uniformly illuminated by light of wavelength $2\pi/k$, as follows. Consider a grating with $4N$ equal strips each of width a and alternately opaque and transparent. The aperture function is then

$$f(y) = \begin{cases} A & \text{for } (2n+1)a \le y \le (2n+2)a, \quad -N \le n < N, \\ 0 & \text{otherwise.} \end{cases}$$

(a) Show, for diffraction at angle θ to the normal to the grating, that the required Fourier transform can be written

$$\tilde{f}(q) = (2\pi)^{-1/2} \sum_{r=-N}^{N-1} \exp(-2iarq) \int_a^{2a} A \exp(-iqu)\, du,$$

where $q = k \sin\theta$.

(b) Evaluate the integral and sum to show that

$$\tilde{f}(q) = (2\pi)^{-1/2} \exp(-iqa/2) \frac{A \sin(2qaN)}{q \cos(qa/2)},$$

and hence that the intensity distribution $I(\theta)$ in the spectrum is proportional to

$$\frac{\sin^2(2qaN)}{q^2 \cos^2(qa/2)}.$$

(c) For large values of N, the numerator in the above expression has very closely spaced maxima and minima as a function of θ and effectively takes its mean value, 1/2, giving a low-intensity background. Much more significant peaks in $I(\theta)$ occur when $\theta = 0$ or the cosine term in the denominator vanishes. Show that the corresponding values of $|\tilde{f}(q)|$ are

$$\frac{2aNA}{(2\pi)^{1/2}} \quad \text{and} \quad \frac{4aNA}{(2\pi)^{1/2}(2m+1)\pi}, \quad \text{with } m \text{ integral.}$$

Note that the constructive interference makes the maxima in $I(\theta) \propto N^2$, not N. Of course, observable maxima only occur for $0 \le \theta \le \pi/2$.

13.9 By finding the complex Fourier *series* for its LHS show that either side of the equation

$$\sum_{n=-\infty}^{\infty} \delta(t + nT) = \frac{1}{T} \sum_{n=-\infty}^{\infty} e^{-2\pi nit/T}$$

can represent a periodic train of impulses. By expressing the function $f(t + nX)$, in which X is a constant, in terms of the Fourier *transform* $\tilde{f}(\omega)$ of $f(t)$, show that

$$\sum_{n=-\infty}^{\infty} f(t + nX) = \frac{\sqrt{2\pi}}{X} \sum_{n=-\infty}^{\infty} \tilde{f}\left(\frac{2n\pi}{X}\right) e^{2\pi nit/X}.$$

This result is known as the *Poisson summation formula.*

13.10 In many applications in which the frequency spectrum of an analogue signal is required, the best that can be done is to sample the signal $f(t)$ a finite number of times at fixed intervals, and then use a *discrete Fourier transform* F_k to estimate discrete points on the (true) frequency spectrum $\tilde{f}(\omega)$.

(a) By an argument that is essentially the converse of that given in section 13.1, show that, if N samples f_n, beginning at $t = 0$ and spaced τ apart, are taken, then $\tilde{f}(2\pi k/(N\tau)) \approx F_k\tau$ where

$$F_k = \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{N-1} f_n e^{-2\pi nki/N}.$$

(b) For the function $f(t)$ defined by

$$f(t) = \begin{cases} 1 & \text{for } 0 \le t < 1, \\ 0 & \text{otherwise,} \end{cases}$$

from which eight samples are drawn at intervals of $\tau = 0.25$, find a formula for $|F_k|$ and evaluate it for $k = 0, 1, \ldots, 7$.

(c) Find the exact frequency spectrum of $f(t)$ and compare the actual and estimated values of $\sqrt{2\pi}|\tilde{f}(\omega)|$ at $\omega = k\pi$ for $k = 0, 1, \ldots, 7$. Note the relatively good agreement for $k < 4$ and the lack of agreement for larger values of k.

13.11 For a function $f(t)$ that is non-zero only in the range $|t| < T/2$, the full frequency spectrum $\tilde{f}(\omega)$ can be constructed, in principle exactly, from values at discrete sample points $\omega = n(2\pi/T)$. Prove this as follows.

(a) Show that the coefficients of a complex Fourier *series* representation of $f(t)$ with period T can be written as

$$c_n = \frac{\sqrt{2\pi}}{T}\tilde{f}\left(\frac{2\pi n}{T}\right).$$

(b) Use this result to represent $f(t)$ as an infinite sum in the defining integral for $\tilde{f}(\omega)$, and hence show that

$$\tilde{f}(\omega) = \sum_{n=-\infty}^{\infty} \tilde{f}\left(\frac{2\pi n}{T}\right) \operatorname{sinc}\left(n\pi - \frac{\omega T}{2}\right),$$

where sinc x is defined as $(\sin x)/x$.

13.12 A signal obtained by sampling a function $x(t)$ at regular intervals T is passed through an electronic filter, whose response $g(t)$ to a unit δ-function input is represented in a tg-plot by straight lines joining $(0, 0)$ to $(T, 1/T)$ to $(2T, 0)$ and is zero for all other values of t. The output of the filter is the convolution of the input, $\sum_{-\infty}^{\infty} x(t)\delta(t - nT)$, with $g(t)$.
Using the convolution theorem, and the result given in exercise 13.4, show that the output of the filter can be written

$$y(t) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} x(nT) \int_{-\infty}^{\infty} \operatorname{sinc}^2\left(\frac{\omega T}{2}\right) e^{-i\omega[(n+1)T - t]}\, d\omega.$$

13.13 Find the Fourier transform specified in part (a) and then use it to answer part (b).

(a) Find the Fourier transform of

$$f(\gamma, p, t) = \begin{cases} e^{-\gamma t} \sin pt & t > 0, \\ 0 & t < 0, \end{cases}$$

where γ (> 0) and p are constant parameters.

(b) The current $I(t)$ flowing through a certain system is related to the applied voltage $V(t)$ by the equation

$$I(t) = \int_{-\infty}^{\infty} K(t-u)V(u)\,du,$$

where

$$K(\tau) = a_1 f(\gamma_1, p_1, \tau) + a_2 f(\gamma_2, p_2, \tau).$$

The function $f(\gamma, p, t)$ is as given in (a) and all the a_i, γ_i (> 0) and p_i are fixed parameters. By considering the Fourier transform of $I(t)$, find the relationship that must hold between a_1 and a_2 if the total net charge Q passed through the system (over a very long time) is to be zero for an arbitrary applied voltage.

13.14 Prove the equality

$$\int_0^{\infty} e^{-2at} \sin^2 at\,dt = \frac{1}{\pi} \int_0^{\infty} \frac{a^2}{4a^4 + \omega^4}\,d\omega.$$

13.15 A linear amplifier produces an output that is the convolution of its input and its response function. The Fourier transform of the response function for a particular amplifier is

$$\tilde{K}(\omega) = \frac{i\omega}{\sqrt{2\pi}(\alpha + i\omega)^2}.$$

Determine the time variation of its output $g(t)$ when its input is the Heaviside step function. (Consider the Fourier transform of a decaying exponential function and the result of exercise 13.2(b).)

13.16 In quantum mechanics, two equal-mass particles having momenta $\mathbf{p}_j = \hbar\mathbf{k}_j$ and energies $E_j = \hbar\omega_j$ and represented by plane wavefunctions $\phi_j = \exp[i(\mathbf{k}_j \cdot \mathbf{r}_j - \omega_j t)]$, $j = 1, 2$, interact through a potential $V = V(|\mathbf{r}_1 - \mathbf{r}_2|)$. In first-order perturbation theory the probability of scattering to a state with momenta and energies $\mathbf{p}'_j, E'_j$ is determined by the modulus squared of the quantity

$$M = \iiint \psi_{\rm f}^* V \psi_{\rm i}\,d\mathbf{r}_1\,d\mathbf{r}_2\,dt.$$

The initial state, $\psi_{\rm i}$, is $\phi_1\phi_2$ and the final state, $\psi_{\rm f}$, is $\phi'_1\phi'_2$.

(a) By writing $\mathbf{r}_1 + \mathbf{r}_2 = 2\mathbf{R}$ and $\mathbf{r}_1 - \mathbf{r}_2 = \mathbf{r}$ and assuming that $d\mathbf{r}_1\,d\mathbf{r}_2 = d\mathbf{R}\,d\mathbf{r}$, show that M can be written as the product of three one-dimensional integrals.

(b) From two of the integrals deduce energy and momentum conservation in the form of δ-functions.

(c) Show that M is proportional to the Fourier transform of V, i.e. to $\widetilde{V}(\mathbf{k})$ where $2\hbar\mathbf{k} = (\mathbf{p}_2 - \mathbf{p}_1) - (\mathbf{p}'_2 - \mathbf{p}'_1)$ or, alternatively, $\hbar\mathbf{k} = \mathbf{p}'_1 - \mathbf{p}_1$.

13.17 For some ion–atom scattering processes, the potential V of the previous exercise may be approximated by $V = |\mathbf{r}_1 - \mathbf{r}_2|^{-1} \exp(-\mu|\mathbf{r}_1 - \mathbf{r}_2|)$. Show, using the result of the worked example in subsection 13.1.10, that the probability that the ion will scatter from, say, $\mathbf{p}_1$ to $\mathbf{p}'_1$ is proportional to $(\mu^2 + k^2)^{-2}$, where $k = |\mathbf{k}|$ and $\mathbf{k}$ is as given in part (c) of that exercise.

13.18 The equivalent duration and bandwidth, T_e and B_e, of a signal $x(t)$ are defined in terms of the latter and its Fourier transform $\tilde{x}(\omega)$ by

$$T_e = \frac{1}{x(0)} \int_{-\infty}^{\infty} x(t)\, dt,$$
$$B_e = \frac{1}{\tilde{x}(0)} \int_{-\infty}^{\infty} \tilde{x}(\omega)\, d\omega,$$

where neither $x(0)$ nor $\tilde{x}(0)$ is zero. Show that the product $T_e B_e = 2\pi$ (this is a form of uncertainty principle), and find the equivalent bandwidth of the signal

$$x(t) = \exp(-|t|/T).$$

For this signal, determine the fraction of the total energy that lies in the frequency range $|\omega| < B_e/4$. You will need the indefinite integral with respect to x of $(a^2 + x^2)^{-2}$, which is

$$\frac{x}{2a^2(a^2 + x^2)} + \frac{1}{2a^3} \tan^{-1} \frac{x}{a}.$$

13.19 Calculate directly the auto-correlation function $a(z)$ for the product $f(t)$ of the exponential decay distribution and the Heaviside step function,

$$f(t) = \frac{1}{\lambda} e^{-\lambda t} H(t).$$

Use the Fourier transform and energy spectrum of $f(t)$ to deduce that

$$\int_{-\infty}^{\infty} \frac{e^{i\omega z}}{\lambda^2 + \omega^2}\, d\omega = \frac{\pi}{\lambda} e^{-\lambda |z|}.$$

13.20 Prove that the cross-correlation $C(z)$ of the Gaussian and Lorentzian distributions

$$f(t) = \frac{1}{\tau\sqrt{2\pi}} \exp\left(-\frac{t^2}{2\tau^2}\right), \qquad g(t) = \left(\frac{a}{\pi}\right) \frac{1}{t^2 + a^2},$$

has as its Fourier transform the function

$$\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\tau^2\omega^2}{2}\right) \exp(-a|\omega|).$$

Hence show that

$$C(z) = \frac{1}{\tau\sqrt{2\pi}} \exp\left(\frac{a^2 - z^2}{2\tau^2}\right) \cos\left(\frac{az}{\tau^2}\right).$$

13.21 Prove the expressions given in table 13.1 for the Laplace transforms of $t^{-1/2}$ and $t^{1/2}$, by setting $x^2 = ts$ in the result

$$\int_0^{\infty} \exp(-x^2)\, dx = \tfrac{1}{2}\sqrt{\pi}.$$

13.22 Find the functions $y(t)$ whose Laplace transforms are the following:

(a) $1/(s^2 - s - 2)$;
(b) $2s/[(s+1)(s^2+4)]$;
(c) $e^{-(\gamma+s)t_0}/[(s+\gamma)^2 + b^2]$.

13.23 Use the properties of Laplace transforms to prove the following without evaluating any Laplace integrals explicitly:

(a) $\mathscr{L}\left[t^{5/2}\right] = \frac{15}{8}\sqrt{\pi} s^{-7/2}$;
(b) $\mathscr{L}\left[(\sinh at)/t\right] = \frac{1}{2} \ln\left[(s+a)/(s-a)\right], \qquad s > |a|$;

(c) $\mathscr{L}[\sinh at \cos bt] = a(s^2 - a^2 + b^2)[(s-a)^2 + b^2]^{-1}[(s+a)^2 + b^2]^{-1}$.

13.24 Find the solution (the so-called *impulse response* or *Green's function*) of the equation

$$T\frac{dx}{dt} + x = \delta(t)$$

by proceeding as follows.

(a) Show by substitution that

$$x(t) = A(1 - e^{-t/T})H(t)$$

is a solution, for which $x(0) = 0$, of

$$T\frac{dx}{dt} + x = AH(t), \qquad (*)$$

where $H(t)$ is the Heaviside step function.

(b) Construct the solution when the RHS of $(*)$ is replaced by $AH(t-\tau)$, with $dx/dt = x = 0$ for $t < \tau$, and hence find the solution when the RHS is a rectangular pulse of duration τ.

(c) By setting $A = 1/\tau$ and taking the limit as $\tau \to 0$, show that the impulse response is $x(t) = T^{-1}e^{-t/T}$.

(d) Obtain the same result much more directly by taking the Laplace transform of each term in the original equation, solving the resulting algebraic equation and then using the entries in table 13.1.

13.25 This exercise is concerned with the limiting behaviour of Laplace transforms.

(a) If $f(t) = A + g(t)$, where A is a constant and the indefinite integral of $g(t)$ is bounded as its upper limit tends to ∞, show that

$$\lim_{s\to 0} s\bar{f}(s) = A.$$

(b) For $t > 0$, the function $y(t)$ obeys the differential equation

$$\frac{d^2y}{dt^2} + a\frac{dy}{dt} + by = c\cos^2\omega t,$$

where a, b and c are positive constants. Find $\bar{y}(s)$ and show that $s\bar{y}(s) \to c/2b$ as $s \to 0$. Interpret the result in the t-domain.

13.26 By writing $f(x)$ as an integral involving the δ-function $\delta(\xi - x)$ and taking the Laplace transforms of both sides, show that the transform of the solution of the equation

$$\frac{d^4y}{dx^4} - y = f(x)$$

for which y and its first three derivatives vanish at $x = 0$ can be written as

$$\bar{y}(s) = \int_0^\infty f(\xi)\frac{e^{-s\xi}}{s^4 - 1}\,d\xi.$$

Use the properties of Laplace transforms and the entries in table 13.1 to show that

$$y(x) = \frac{1}{2}\int_0^x f(\xi)\left[\sinh(x-\xi) - \sin(x-\xi)\right]\,d\xi.$$

13.27 The function $f_a(x)$ is defined as unity for $0 < x < a$ and zero otherwise. Find its Laplace transform $\bar{f}_a(s)$ and deduce that the transform of $xf_a(x)$ is

$$\frac{1}{s^2}\left[1-(1+as)e^{-sa}\right].$$

Write $f_a(x)$ in terms of Heaviside functions and hence obtain an explicit expression for

$$g_a(x) = \int_0^x f_a(y)f_a(x-y)\,dy.$$

Use the expression to write $\bar{g}_a(s)$ in terms of the functions $\bar{f}_a(s)$ and $\bar{f}_{2a}(s)$, and their derivatives, and hence show that $\bar{g}_a(s)$ is equal to the square of $\bar{f}_a(s)$, in accordance with the convolution theorem.

13.28 Show that the Laplace transform of $f(t-a)H(t-a)$, where $a \geq 0$, is $e^{-as}\bar{f}(s)$ and that, if $g(t)$ is a periodic function of period T, $\bar{g}(s)$ can be written as

$$\frac{1}{1-e^{-sT}}\int_0^T e^{-st}g(t)\,dt.$$

(a) Sketch the periodic function defined in $0 \leq t \leq T$ by

$$g(t) = \begin{cases} 2t/T & 0 \leq t < T/2, \\ 2(1-t/T) & T/2 \leq t \leq T, \end{cases}$$

and, using the previous result, find its Laplace transform.

(b) Show, by sketching it, that

$$\frac{2}{T}[tH(t) + 2\sum_{n=1}^{\infty}(-1)^n(t-\tfrac{1}{2}nT)H(t-\tfrac{1}{2}nT)]$$

is another representation of $g(t)$ and hence derive the relationship

$$\tanh x = 1 + 2\sum_{n=1}^{\infty}(-1)^n e^{-2nx}.$$

13.5 Hints and answers

13.1 Note that the integrand has different analytic forms for $t < 0$ and $t \geq 0$. $(2/\pi)^{1/2}(1+\omega^2)^{-1}$.

13.3 $(1/\sqrt{2\pi})[(b-ik)/(b^2+k^2)]e^{-a(b+ik)}$.

13.5 Use or derive $\widetilde{\phi''}(k) = -k^2\tilde{\phi}(k)$ to obtain an algebraic equation for $\tilde{\phi}(k)$ and then use the Fourier inversion formula.

13.7 $(2/\sqrt{2\pi})(\sin\omega/\omega)$.
The convolution is $2-|t|$ for $|t| < 2$, zero otherwise. Use the convolution theorem.
$(4/\sqrt{2\pi})(\sin^2\omega/\omega^2)$.
Apply Parseval's theorem to f and to $f * f$.

13.9 The Fourier coefficient is T^{-1}, independent of n. Make the changes of variables $t \to \omega$, $n \to -n$ and $T \to 2\pi/X$ and apply the translation theorem.

13.11 (b) Recall that the infinite integral involved in defining $\tilde{f}(\omega)$ has a non-zero integrand only in $|t| < T/2$.

13.13 (a) $(1/\sqrt{2\pi})\{p/[(\gamma+i\omega)^2+p^2]\}$.
(b) Show that $Q = \sqrt{2\pi}\tilde{I}(0)$ and use the convolution theorem. The required relationship is $a_1p_1/(\gamma_1^2+p_1^2) + a_2p_2/(\gamma_2^2+p_2^2) = 0$.

13.15 $\tilde{g}(\omega) = 1/[\sqrt{2\pi}(\alpha+i\omega)^2]$, leading to $g(t) = te^{-\alpha t}$.

13.17 $\widetilde{V}(\mathbf{k}) \propto [-2\pi/(ik)] \int \{\exp[-(\mu - ik)r] - \exp[-(\mu + ik)r]\} \, dr$.

13.19 Note that the lower limit in the calculation of $a(z)$ is 0, for $z > 0$, and $|z|$, for $z < 0$. Auto-correlation $a(z) = [(1/(2\lambda^3)] \exp(-\lambda|z|)$.

13.21 Prove the result for $t^{1/2}$ by integrating that for $t^{-1/2}$ by parts.

13.23 (a) Use (13.62) with $n = 2$ on $\mathscr{L}\left[\sqrt{t}\right]$; (b) use (13.63); (c) consider $\mathscr{L}$ $[\exp(\pm at) \cos bt]$ and use the translation property, subsection 13.2.2.

13.25 (a) Note that $|\lim \int g(t)e^{-st} \, dt| \leq |\lim \int g(t) \, dt|$.
(b) $(s^2 + as + b)\bar{y}(s) = \{c(s^2 + 2\omega^2)/[s(s^2 + 4\omega^2)]\} + (a + s)y(0) + y'(0)$.
For this damped system, at large t (corresponding to $s \to 0$) rates of change are negligible and the equation reduces to $by = c \cos^2 \omega t$. The average value of $\cos^2 \omega t$ is $\frac{1}{2}$.

13.27 $s^{-1}[1 - \exp(-sa)]$; $g_a(x) = x$ for $0 < x < a$, $g_a(x) = 2a - x$ for $a \leq x \leq 2a$, $g_a(x) = 0$ otherwise.

14

First-order ordinary differential equations

Differential equations are the group of equations that contain derivatives. Chapters 14–21 discuss a variety of differential equations, starting in this chapter and the next with those ordinary differential equations (ODEs) that have closed-form solutions. As its name suggests, an ODE contains only ordinary derivatives (no partial derivatives) and describes the relationship between these derivatives of the *dependent variable*, usually called y, with respect to the *independent variable*, usually called x. The solution to such an ODE is therefore a function of x and is written $y(x)$. For an ODE to have a closed-form solution, it must be possible to express $y(x)$ in terms of the standard elementary functions such as $\exp x$, $\ln x$, $\sin x$ etc. The solutions of some differential equations cannot, however, be written in closed form, but only as an infinite series; these are discussed in chapter 16.

Ordinary differential equations may be separated conveniently into different categories according to their general characteristics. The primary grouping adopted here is by the *order* of the equation. The order of an ODE is simply the order of the highest derivative it contains. Thus equations containing dy/dx, but no higher derivatives, are called first order, those containing d^2y/dx^2 are called second order and so on. In this chapter we consider first-order equations, and in the next, second- and higher-order equations.

Ordinary differential equations may be classified further according to *degree*. The degree of an ODE is the power to which the highest-order derivative is raised, after the equation has been rationalised to contain only integer powers of derivatives. Hence the ODE

$$\frac{d^3y}{dx^3} + x\left(\frac{dy}{dx}\right)^{3/2} + x^2y = 0,$$

is of third order and second degree, since after rationalisation it contains the term $(d^3y/dx^3)^2$.

The *general solution* to an ODE is the most general function $y(x)$ that satisfies the equation; it will contain *constants of integration* which may be determined by the application of some suitable *boundary conditions*. For example, we may be told that for a certain first-order differential equation, the solution $y(x)$ is equal to zero when the parameter x is equal to unity; this allows us to determine the value of the constant of integration. The *general solutions* to nth-order ODEs, which are considered in detail in the next chapter, will contain n (essential) arbitrary constants of integration and therefore we will need n boundary conditions if these constants are to be determined (see section 14.1). When the boundary conditions have been applied, and the constants found, we are left with a *particular solution* to the ODE, which obeys the given boundary conditions. Some ODEs of degree greater than unity also possess *singular solutions*, which are solutions that contain no arbitrary constants and cannot be found from the general solution; singular solutions are discussed in more detail in section 14.3. When any solution to an ODE has been found, it is always possible to check its validity by substitution into the original equation and verification that any given boundary conditions are met.

In this chapter, firstly we discuss various types of first-degree ODE and then go on to examine those higher-degree equations that can be solved in closed form. At the outset, however, we discuss the general form of the solutions of ODEs; this discussion is relevant to both first- and higher-order ODEs.

14.1 General form of solution

It is helpful when considering the general form of the solution of an ODE to consider the inverse process, namely that of obtaining an ODE from a given group of functions, each one of which is a solution of the ODE. Suppose the members of the group can be written as

$$y = f(x, a_1, a_2, \ldots, a_n), \tag{14.1}$$

each member being specified by a different set of values of the parameters a_i. For example, consider the group of functions

$$y = a_1 \sin x + a_2 \cos x; \tag{14.2}$$

here $n = 2$.

Since an ODE is required for which *any* of the group is a solution, it clearly must not contain any of the a_i. As there are n of the a_i in expression (14.1), we must obtain $n + 1$ equations involving them in order that, by elimination, we can obtain one final equation without them.

Initially we have only (14.1), but if this is differentiated n times, a total of $n + 1$ equations is obtained from which (in principle) all the a_i can be eliminated, to give one ODE satisfied by all the group. As a result of the n differentiations, $d^n y/dx^n$ will be present in one of the $n + 1$ equations and hence in the final equation, which will therefore be of nth order.

In the case of (14.2), we have

$$\frac{dy}{dx} = a_1 \cos x - a_2 \sin x,$$
$$\frac{d^2y}{dx^2} = -a_1 \sin x - a_2 \cos x.$$

Here the elimination of a_1 and a_2 is trivial (because of the similarity of the forms of y and d^2y/dx^2), resulting in

$$\frac{d^2y}{dx^2} + y = 0,$$

a second-order equation.

Thus, to summarise, a group of functions (14.1) with n parameters satisfies an nth-order ODE in general (although in some degenerate cases an ODE of less than nth order is obtained). The intuitive converse of this is that the general solution of an nth-order ODE contains n arbitrary parameters (constants); for our purposes, this will be assumed to be valid although a totally general proof is difficult.

As mentioned earlier, external factors affect a system described by an ODE, by fixing the values of the dependent variables for particular values of the independent ones. These externally imposed (or *boundary*) conditions on the solution are thus the means of determining the parameters and so of specifying precisely which function is the required solution. It is apparent that the number of boundary conditions should match the number of parameters and hence the order of the equation, if a unique solution is to be obtained. Fewer independent boundary conditions than this will lead to a number of undetermined parameters in the solution, whilst an excess will usually mean that no acceptable solution is possible.

For an nth-order equation the required n boundary conditions can take many forms, for example the value of y at n different values of x, or the value of any $n-1$ of the n derivatives dy/dx, d^2y/dx^2, …, d^ny/dx^n together with that of y, all for the same value of x, or many intermediate combinations.

14.2 First-degree first-order equations

First-degree first-order ODEs contain only dy/dx equated to some function of x and y, and can be written in either of two equivalent standard forms,

$$\frac{dy}{dx} = F(x,y), \qquad A(x,y)\,dx + B(x,y)\,dy = 0,$$

where $F(x,y) = -A(x,y)/B(x,y)$, and $F(x,y)$, $A(x,y)$ and $B(x,y)$ are in general functions of both x and y. Which of the two above forms is the more useful for finding a solution depends on the type of equation being considered. There are several different types of first-degree first-order ODEs that are of interest in the physical sciences. These equations and their respective solutions are discussed below.

14.2.1 Separable-variable equations

A separable-variable equation is one which may be written in the conventional form

$$\frac{dy}{dx} = f(x)g(y), \tag{14.3}$$

where $f(x)$ and $g(y)$ are functions of x and y respectively, including cases in which $f(x)$ or $g(y)$ is simply a constant. Rearranging this equation so that the terms depending on x and on y appear on opposite sides (i.e. are separated), and integrating, we obtain

$$\int \frac{dy}{g(y)} = \int f(x)\, dx.$$

Finding the solution $y(x)$ that satisfies (14.3) then depends only on the ease with which the integrals in the above equation can be evaluated. It is also worth noting that ODEs that at first sight do not appear to be of the form (14.3) can sometimes be made separable by an appropriate factorisation.

►*Solve*

$$\frac{dy}{dx} = x + xy.$$

Since the RHS of this equation can be factorised to give $x(1 + y)$, the equation becomes separable and we obtain

$$\int \frac{dy}{1+y} = \int x\, dx.$$

Now integrating both sides separately, we find

$$\ln(1 + y) = \frac{x^2}{2} + c,$$

and so

$$1 + y = \exp\left(\frac{x^2}{2} + c\right) = A \exp\left(\frac{x^2}{2}\right),$$

where c and hence A is an arbitrary constant. ◄

Solution method. *Factorise the equation so that it becomes separable. Rearrange it so that the terms depending on x and those depending on y appear on opposite sides and then integrate directly. Remember the constant of integration, which can be evaluated if further information is given.*

14.2.2 Exact equations

An *exact* first-degree first-order ODE is one of the form

$$A(x,y)\,dx + B(x,y)\,dy = 0 \quad \text{and for which} \quad \frac{\partial A}{\partial y} = \frac{\partial B}{\partial x}. \tag{14.4}$$

In this case $A(x,y)\,dx + B(x,y)\,dy$ is an exact differential, $dU(x,y)$ say (see section 5.3). In other words

$$A\,dx + B\,dy = dU = \frac{\partial U}{\partial x}\,dx + \frac{\partial U}{\partial y}\,dy,$$

from which we obtain

$$A(x,y) = \frac{\partial U}{\partial x}, \tag{14.5}$$

$$B(x,y) = \frac{\partial U}{\partial y}. \tag{14.6}$$

Since $\partial^2 U/\partial x \partial y = \partial^2 U/\partial y \partial x$ we therefore require

$$\frac{\partial A}{\partial y} = \frac{\partial B}{\partial x}. \tag{14.7}$$

If (14.7) holds then (14.4) can be written $dU(x,y) = 0$, which has the solution $U(x,y) = c$, where c is a constant and from (14.5) $U(x,y)$ is given by

$$U(x,y) = \int A(x,y)\,dx + F(y). \tag{14.8}$$

The function $F(y)$ can be found from (14.6) by differentiating (14.8) with respect to y and equating to $B(x,y)$.

►*Solve*

$$x\frac{dy}{dx} + 3x + y = 0.$$

Rearranging into the form (14.4) we have

$$(3x + y)\,dx + x\,dy = 0,$$

i.e. $A(x,y) = 3x + y$ and $B(x,y) = x$. Since $\partial A/\partial y = 1 = \partial B/\partial x$, the equation is exact, and by (14.8) the solution is given by

$$U(x,y) = \int (3x + y)\,dx + F(y) = c_1 \quad \Rightarrow \quad \frac{3x^2}{2} + yx + F(y) = c_1.$$

Differentiating $U(x,y)$ with respect to y and equating it to $B(x,y) = x$ we obtain $dF/dy = 0$, which integrates immediately to give $F(y) = c_2$. Therefore, letting $c = c_1 - c_2$, the solution to the original ODE is

$$\frac{3x^2}{2} + xy = c. \blacktriangleleft$$

Solution method. *Check that the equation is an exact differential using (14.7) then solve using (14.8). Find the function $F(y)$ by differentiating (14.8) with respect to y and using (14.6).*

14.2.3 Inexact equations: integrating factors

Equations that may be written in the form

$$A(x,y)\,dx + B(x,y)\,dy = 0 \quad \text{but for which} \quad \frac{\partial A}{\partial y} \neq \frac{\partial B}{\partial x} \tag{14.9}$$

are known as inexact equations. However, the differential $A\,dx + B\,dy$ can always be made exact by multiplying by an *integrating factor* $\mu(x,y)$, which obeys

$$\frac{\partial(\mu A)}{\partial y} = \frac{\partial(\mu B)}{\partial x}. \tag{14.10}$$

For an integrating factor that is a function of both x and y, i.e. $\mu = \mu(x,y)$, there exists no general method for finding it; in such cases it may sometimes be found by inspection. If, however, an integrating factor exists that is a function of either x or y alone then (14.10) can be solved to find it. For example, if we assume that the integrating factor is a function of x alone, i.e. $\mu = \mu(x)$, then (14.10) reads

$$\mu\frac{\partial A}{\partial y} = \mu\frac{\partial B}{\partial x} + B\frac{d\mu}{dx}.$$

Rearranging this expression we find

$$\frac{d\mu}{\mu} = \frac{1}{B}\left(\frac{\partial A}{\partial y} - \frac{\partial B}{\partial x}\right)dx = f(x)\,dx,$$

where we require $f(x)$ also to be a function of x only; indeed this provides a general method of determining whether the integrating factor μ is a function of x alone. This integrating factor is then given by

$$\mu(x) = \exp\left\{\int f(x)\,dx\right\} \quad \text{where} \quad f(x) = \frac{1}{B}\left(\frac{\partial A}{\partial y} - \frac{\partial B}{\partial x}\right). \tag{14.11}$$

Similarly, if $\mu = \mu(y)$ then

$$\mu(y) = \exp\left\{\int g(y)\,dy\right\} \quad \text{where} \quad g(y) = \frac{1}{A}\left(\frac{\partial B}{\partial x} - \frac{\partial A}{\partial y}\right). \tag{14.12}$$

►*Solve*
$$\frac{dy}{dx} = -\frac{2}{y} - \frac{3y}{2x}.$$

Rearranging into the form (14.9), we have
$$(4x + 3y^2)\,dx + 2xy\,dy = 0, \tag{14.13}$$
i.e. $A(x, y) = 4x + 3y^2$ and $B(x, y) = 2xy$. Now
$$\frac{\partial A}{\partial y} = 6y, \qquad \frac{\partial B}{\partial x} = 2y,$$
so the ODE is not exact in its present form. However, we see that
$$\frac{1}{B}\left(\frac{\partial A}{\partial y} - \frac{\partial B}{\partial x}\right) = \frac{2}{x},$$
a function of x alone. Therefore an integrating factor exists that is also a function of x alone and, ignoring the arbitrary constant of integration, is given by
$$\mu(x) = \exp\left\{2\int \frac{dx}{x}\right\} = \exp(2\ln x) = x^2.$$
Multiplying (14.13) through by $\mu(x) = x^2$ we obtain
$$(4x^3 + 3x^2y^2)\,dx + 2x^3y\,dy = 4x^3\,dx + (3x^2y^2\,dx + 2x^3y\,dy) = 0.$$
By inspection this integrates immediately to give the solution $x^4 + y^2x^3 = c$, where c is a constant. ◄

Solution method. *Examine whether $f(x)$ and $g(y)$ are functions of only x or y respectively. If so, then the required integrating factor is a function of either x or y only, and is given by (14.11) or (14.12) respectively. If the integrating factor is a function of both x and y, then sometimes it may be found by inspection or by trial and error. In any case, the integrating factor μ must satisfy (14.10). Once the equation has been made exact, solve by the method of subsection 14.2.2.*

14.2.4 Linear equations

Linear first-order ODEs are a special case of inexact ODEs (discussed in the previous subsection) and can be written in the conventional form
$$\frac{dy}{dx} + P(x)y = Q(x). \tag{14.14}$$
Such equations can be made exact by multiplying through by an appropriate integrating factor in a similar manner to that discussed above. In this case, however, the integrating factor is always a function of x alone and may be expressed in a particularly simple form. An integrating factor $\mu(x)$ must be such that
$$\mu(x)\frac{dy}{dx} + \mu(x)P(x)y = \frac{d}{dx}\left[\mu(x)y\right] = \mu(x)Q(x), \tag{14.15}$$

which may then be integrated directly to give

$$\mu(x)y = \int \mu(x)Q(x)\,dx. \tag{14.16}$$

The required integrating factor $\mu(x)$ is determined by the first equality in (14.15), i.e.

$$\frac{d}{dx}(\mu y) = \mu\frac{dy}{dx} + \frac{d\mu}{dx}y = \mu\frac{dy}{dx} + \mu P y,$$

which immediately gives the simple relation

$$\frac{d\mu}{dx} = \mu(x)P(x) \qquad \Rightarrow \qquad \mu(x) = \exp\left\{\int P(x)\,dx\right\}. \tag{14.17}$$

►*Solve*

$$\frac{dy}{dx} + 2xy = 4x.$$

The integrating factor is given immediately by

$$\mu(x) = \exp\left\{\int 2x\,dx\right\} = \exp x^2.$$

Multiplying through the ODE by $\mu(x) = \exp x^2$ and integrating, we have

$$y\exp x^2 = 4\int x\exp x^2\,dx = 2\exp x^2 + c.$$

The solution to the ODE is therefore given by $y = 2 + c\exp(-x^2)$. ◄

Solution method. *Rearrange the equation into the form (14.14) and multiply by the integrating factor $\mu(x)$ given by (14.17). The left- and right-hand sides can then be integrated directly, giving y from (14.16).*

14.2.5 Homogeneous equations

Homogeneous equation are ODEs that may be written in the form

$$\frac{dy}{dx} = \frac{A(x,y)}{B(x,y)} = F\left(\frac{y}{x}\right), \tag{14.18}$$

where $A(x,y)$ and $B(x,y)$ are homogeneous functions of the same degree. A function $f(x,y)$ is homogeneous of degree n if, for any λ, it obeys

$$f(\lambda x, \lambda y) = \lambda^n f(x,y).$$

For example, if $A = x^2y - xy^2$ and $B = x^3 + y^3$ then we see that A and B are both homogeneous functions of degree 3. In general, for functions of the form of A and B, we see that for both to be homogeneous, and of the same degree, we require the sum of the powers in x and y in each term of A and B to be the same (in this example equal to 3). The RHS of a homogeneous ODE can be written as a function of y/x. The equation may then be solved by making the substitution $y = vx$, so that

$$\frac{dy}{dx} = v + x\frac{dv}{dx} = F(v).$$

This is now a separable equation and can be integrated directly to give

$$\int \frac{dv}{F(v) - v} = \int \frac{dx}{x}. \tag{14.19}$$

►*Solve*

$$\frac{dy}{dx} = \frac{y}{x} + \tan\left(\frac{y}{x}\right).$$

Substituting $y = vx$ we obtain

$$v + x\frac{dv}{dx} = v + \tan v.$$

Cancelling v on both sides, rearranging and integrating gives

$$\int \cot v \, dv = \int \frac{dx}{x} = \ln x + c_1.$$

But

$$\int \cot v \, dv = \int \frac{\cos v}{\sin v} \, dv = \ln(\sin v) + c_2,$$

so the solution to the ODE is $y = x \sin^{-1} Ax$, where A is a constant. ◄

Solution method. *Check to see whether the equation is homogeneous. If so, make the substitution $y = vx$, separate variables as in (14.19) and then integrate directly. Finally replace v by y/x to obtain the solution.*

14.2.6 Isobaric equations

An isobaric ODE is a generalisation of the homogeneous ODE discussed in the previous section, and is of the form

$$\frac{dy}{dx} = \frac{A(x, y)}{B(x, y)}, \tag{14.20}$$

where the equation is dimensionally consistent if y and dy are each given a weight m relative to x and dx, i.e. if the substitution $y = vx^m$ makes it separable.

►*Solve*

$$\frac{dy}{dx} = \frac{-1}{2yx}\left(y^2 + \frac{2}{x}\right).$$

Rearranging we have

$$\left(y^2 + \frac{2}{x}\right) dx + 2yx\, dy = 0.$$

Giving y and dy the weight m and x and dx the weight 1, the sums of the powers in each term on the LHS are $2m+1$, 0 and $2m+1$ respectively. These are equal if $2m+1=0$, i.e. if $m=-\frac{1}{2}$. Substituting $y = vx^m = vx^{-1/2}$, with the result that $dy = x^{-1/2}\,dv - \frac{1}{2}vx^{-3/2}\,dx$, we obtain

$$v\,dv + \frac{dx}{x} = 0,$$

which is separable and may be integrated directly to give $\frac{1}{2}v^2 + \ln x = c$. Replacing v by $y\sqrt{x}$ we obtain the solution $\frac{1}{2}y^2x + \ln x = c$. ◄

Solution method. *Write the equation in the form $A\,dx + B\,dy = 0$. Giving y and dy each a weight m and x and dx each a weight 1, write down the sum of powers in each term. Then, if a value of m that makes all these sums equal can be found, substitute $y = vx^m$ into the original equation to make it separable. Integrate the separated equation directly, and then replace v by yx^{-m} to obtain the solution.*

14.2.7 Bernoulli's equation

Bernoulli's equation has the form

$$\frac{dy}{dx} + P(x)y = Q(x)y^n \quad \text{where } n \neq 0 \text{ or } 1. \tag{14.21}$$

This equation is very similar in form to the linear equation (14.14), but is in fact non-linear due to the extra y^n factor on the RHS. However, the equation can be made linear by substituting $v = y^{1-n}$ and correspondingly

$$\frac{dy}{dx} = \left(\frac{y^n}{1-n}\right)\frac{dv}{dx}.$$

Substituting this into (14.21) and dividing through by y^n, we find

$$\frac{dv}{dx} + (1-n)P(x)v = (1-n)Q(x),$$

which is a linear equation and may be solved by the method described in subsection 14.2.4.

►*Solve*

$$\frac{dy}{dx} + \frac{y}{x} = 2x^3y^4.$$

If we let $v = y^{1-4} = y^{-3}$ then

$$\frac{dy}{dx} = -\frac{y^4}{3}\frac{dv}{dx}.$$

Substituting this into the ODE and rearranging, we obtain

$$\frac{dv}{dx} - \frac{3v}{x} = -6x^3,$$

which is linear and may be solved by multiplying through by the integrating factor (see subsection 14.2.4)

$$\exp\left\{-3\int\frac{dx}{x}\right\} = \exp(-3\ln x) = \frac{1}{x^3}.$$

This yields the solution

$$\frac{v}{x^3} = -6x + c.$$

Remembering that $v = y^{-3}$, we obtain $y^{-3} = -6x^4 + cx^3$. ◄

Solution method. *Rearrange the equation into the form (14.21) and make the substitution $v = y^{1-n}$. This leads to a linear equation in v, which can be solved by the method of subsection 14.2.4. Then replace v by y^{1-n} to obtain the solution.*

14.2.8 Miscellaneous equations

There are two further types of first-degree first-order equation that occur fairly regularly but do not fall into any of the above categories. They may be reduced to one of the above equations, however, by a suitable change of variable.

Firstly, we consider

$$\frac{dy}{dx} = F(ax + by + c), \tag{14.22}$$

where a, b and c are constants, i.e. x and y *only* appear on the RHS in the particular combination $ax+by+c$ and not in any other combination or by themselves. This equation can be solved by making the substitution $v = ax + by + c$, in which case

$$\frac{dv}{dx} = a + b\frac{dy}{dx} = a + bF(v), \tag{14.23}$$

which is separable and may be integrated directly.

►*Solve*

$$\frac{dy}{dx} = (x + y + 1)^2.$$

Making the substitution $v = x + y + 1$, we obtain, as in (14.23),

$$\frac{dv}{dx} = v^2 + 1,$$

which is separable and integrates directly to give

$$\int \frac{dv}{1+v^2} = \int dx \quad \Rightarrow \quad \tan^{-1} v = x + c_1.$$

So the solution to the original ODE is $\tan^{-1}(x + y + 1) = x + c_1$, where c_1 is a constant of integration. ◄

Solution method. *In an equation such as (14.22), substitute $v = ax+by+c$ to obtain a separable equation that can be integrated directly. Then replace v by $ax + by + c$ to obtain the solution.*

Secondly, we discuss

$$\frac{dy}{dx} = \frac{ax + by + c}{ex + fy + g}, \tag{14.24}$$

where a, b, c, e, f and g are all constants. This equation may be solved by letting $x = X + \alpha$ and $y = Y + \beta$, where α and β are constants found from

$$a\alpha + b\beta + c = 0 \tag{14.25}$$

$$e\alpha + f\beta + g = 0. \tag{14.26}$$

Then (14.24) can be written as

$$\frac{dY}{dX} = \frac{aX + bY}{eX + fY},$$

which is homogeneous and can be solved by the method of subsection 14.2.5. Note, however, that if $a/e = b/f$ then (14.25) and (14.26) are not independent and so cannot be solved uniquely for α and β. However, in this case, (14.24) reduces to an equation of the form (14.22), which was discussed above.

►*Solve*

$$\frac{dy}{dx} = \frac{2x - 5y + 3}{2x + 4y - 6}.$$

Let $x = X + \alpha$ and $y = Y + \beta$, where α and β obey the relations

$$2\alpha - 5\beta + 3 = 0$$
$$2\alpha + 4\beta - 6 = 0,$$

which solve to give $\alpha = \beta = 1$. Making these substitutions we find

$$\frac{dY}{dX} = \frac{2X - 5Y}{2X + 4Y},$$

which is a homogeneous ODE and can be solved by substituting $Y = vX$ (see subsection 14.2.5) to obtain

$$\frac{dv}{dX} = \frac{2-7v-4v^2}{X(2+4v)}.$$

This equation is separable, and using partial fractions we find

$$\int \frac{2+4v}{2-7v-4v^2}\,dv = -\frac{4}{3}\int \frac{dv}{4v-1} - \frac{2}{3}\int \frac{dv}{v+2} = \int \frac{dX}{X},$$

which integrates to give

$$\ln X + \tfrac{1}{3}\ln(4v-1) + \tfrac{2}{3}\ln(v+2) = c_1,$$

or

$$X^3(4v-1)(v+2)^2 = \exp 3c_1.$$

Remembering that $Y = vX$, $x = X + 1$ and $y = Y + 1$, the solution to the original ODE is given by $(4y - x - 3)(y + 2x - 3)^2 = c_2$, where $c_2 = \exp 3c_1$. ◀

Solution method. *If in (14.24) $a/e \neq b/f$ then make the substitution $x = X + \alpha$, $y = Y + \beta$, where α and β are given by (14.25) and (14.26); the resulting equation is homogeneous and can be solved as in subsection 14.2.5. Substitute $v = Y/X$, $X = x - \alpha$ and $Y = y - \beta$ to obtain the solution. If $a/e = b/f$ then (14.24) is of the same form as (14.22) and may be solved accordingly.*

14.3 Higher-degree first-order equations

First-order equations of degree higher than the first do not occur often in the description of physical systems, since squared and higher powers of first-order derivatives usually arise from resistive or driving mechanisms, when an acceleration or other higher-order derivative is also present. They do sometimes appear in connection with geometrical problems, however.

Higher-degree first-order equations can be written as $F(x, y, dy/dx) = 0$. The most general standard form is

$$p^n + a_{n-1}(x,y)p^{n-1} + \cdots + a_1(x,y)p + a_0(x,y) = 0, \qquad (14.27)$$

where for ease of notation we write $p = dy/dx$. If the equation can be solved for one of x, y or p then either an explicit or a parametric solution can sometimes be obtained. We discuss the main types of such equations below, including Clairaut's equation, which is a special case of an equation explicitly soluble for y.

14.3.1 Equations soluble for p

Sometimes the LHS of (14.27) can be factorised into the form

$$(p - F_1)(p - F_2)\cdots(p - F_n) = 0, \qquad (14.28)$$

where $F_i = F_i(x, y)$. We are then left with solving the n first-degree equations $p = F_i(x, y)$. Writing the solutions to these first-degree equations as $G_i(x, y) = 0$, the general solution to (14.28) is given by the product

$$G_1(x, y)G_2(x, y)\cdots G_n(x, y) = 0. \tag{14.29}$$

►*Solve*

$$(x^3 + x^2 + x + 1)p^2 - (3x^2 + 2x + 1)yp + 2xy^2 = 0. \tag{14.30}$$

This equation may be factorised to give

$$[(x + 1)p - y][(x^2 + 1)p - 2xy] = 0.$$

Taking each bracket in turn we have

$$(x + 1)\frac{dy}{dx} - y = 0,$$
$$(x^2 + 1)\frac{dy}{dx} - 2xy = 0,$$

which have the solutions $y - c(x + 1) = 0$ and $y - c(x^2 + 1) = 0$ respectively (see section 14.2 on first-degree first-order equations). Note that the arbitrary constants in these two solutions can be taken to be the same, since only one is required for a first-order equation. The general solution to (14.30) is then given by

$$[y - c(x + 1)]\left[y - c(x^2 + 1)\right] = 0. \blacktriangleleft$$

Solution method. *If the equation can be factorised into the form (14.28) then solve the first-order ODE* $p - F_i = 0$ *for each factor and write the solution in the form* $G_i(x, y) = 0$. *The solution to the original equation is then given by the product (14.29).*

14.3.2 Equations soluble for x

Equations that can be solved for x, i.e. such that they may be written in the form

$$x = F(y, p), \tag{14.31}$$

can be reduced to first-degree first-order equations in p by differentiating both sides with respect to y, so that

$$\frac{dx}{dy} = \frac{1}{p} = \frac{\partial F}{\partial y} + \frac{\partial F}{\partial p}\frac{dp}{dy}.$$

This results in an equation of the form $G(y, p) = 0$, which can be used together with (14.31) to eliminate p and give the general solution. Note that often a singular solution to the equation will be found at the same time (see the introduction to this chapter).

►*Solve*

$$6y^2p^2 + 3xp - y = 0. \tag{14.32}$$

This equation can be solved for x explicitly to give $3x = (y/p) - 6y^2p$. Differentiating both sides with respect to y, we find

$$3\frac{dx}{dy} = \frac{3}{p} = \frac{1}{p} - \frac{y}{p^2}\frac{dp}{dy} - 6y^2\frac{dp}{dy} - 12yp,$$

which factorises to give

$$\left(1 + 6yp^2\right)\left(2p + y\frac{dp}{dy}\right) = 0. \tag{14.33}$$

Setting the factor containing dp/dy equal to zero gives a first-degree first-order equation in p, which may be solved to give $py^2 = c$. Substituting for p in (14.32) then yields the general solution of (14.32):

$$y^3 = 3cx + 6c^2. \tag{14.34}$$

If we now consider the first factor in (14.33), we find $6p^2y = -1$ as a possible solution. Substituting for p in (14.32) we find the singular solution

$$8y^3 + 3x^2 = 0.$$

Note that the singular solution contains no arbitrary constants and cannot be found from the general solution (14.34) by any choice of the constant c. ◄

Solution method. *Write the equation in the form (14.31) and differentiate both sides with respect to y. Rearrange the resulting equation into the form $G(y, p) = 0$, which can be used together with the original ODE to eliminate p and so give the general solution. If $G(y, p)$ can be factorised then the factor containing dp/dy should be used to eliminate p and give the general solution. Using the other factors in this fashion will instead lead to singular solutions.*

14.3.3 Equations soluble for y

Equations that can be solved for y, i.e. are such that they may be written in the form

$$y = F(x, p), \tag{14.35}$$

can be reduced to first-degree first-order equations in p by differentiating both sides with respect to x, so that

$$\frac{dy}{dx} = p = \frac{\partial F}{\partial x} + \frac{\partial F}{\partial p}\frac{dp}{dx}.$$

This results in an equation of the form $G(x, p) = 0$, which can be used together with (14.35) to eliminate p and give the general solution. An additional (singular) solution to the equation is also often found.

►*Solve*

$$xp^2 + 2xp - y = 0. \tag{14.36}$$

This equation can be solved for y explicitly to give $y = xp^2 + 2xp$. Differentiating both sides with respect to x, we find

$$\frac{dy}{dx} = p = 2xp\frac{dp}{dx} + p^2 + 2x\frac{dp}{dx} + 2p,$$

which after factorising gives

$$(p+1)\left(p + 2x\frac{dp}{dx}\right) = 0. \tag{14.37}$$

To obtain the general solution of (14.36), we consider the factor containing dp/dx. This first-degree first-order equation in p has the solution $xp^2 = c$ (see subsection 14.3.1), which we then use to eliminate p from (14.36). Thus we find that the general solution to (14.36) is

$$(y - c)^2 = 4cx. \tag{14.38}$$

If instead, we set the other factor in (14.37) equal to zero, we obtain the very simple solution $p = -1$. Substituting this into (14.36) then gives

$$x + y = 0,$$

which is a singular solution to (14.36). ◄

Solution method. *Write the equation in the form (14.35) and differentiate both sides with respect to x. Rearrange the resulting equation into the form $G(x, p) = 0$, which can be used together with the original ODE to eliminate p and so give the general solution. If $G(x, p)$ can be factorised then the factor containing dp/dx should be used to eliminate p and give the general solution. Using the other factors in this fashion will instead lead to singular solutions.*

14.3.4 Clairaut's equation

Finally, we consider Clairaut's equation, which has the form

$$y = px + F(p) \tag{14.39}$$

and is therefore a special case of equations soluble for y, as in (14.35). It may be solved by a similar method to that given in subsection 14.3.3, but for Clairaut's equation the form of the general solution is particularly simple. Differentiating (14.39) with respect to x, we find

$$\frac{dy}{dx} = p = p + x\frac{dp}{dx} + \frac{dF}{dp}\frac{dp}{dx} \qquad \Rightarrow \qquad \frac{dp}{dx}\left(\frac{dF}{dp} + x\right) = 0. \tag{14.40}$$

Considering first the factor containing dp/dx, we find

$$\frac{dp}{dx} = \frac{d^2y}{dx^2} = 0 \qquad \Rightarrow \qquad y = c_1x + c_2. \tag{14.41}$$

Since $p = dy/dx = c_1$, if we substitute (14.41) into (14.39) we find $c_1 x + c_2 = c_1 x + F(c_1)$. Therefore the constant c_2 is given by $F(c_1)$, and the general solution to (14.39) is

$$y = c_1 x + F(c_1), \tag{14.42}$$

i.e. the general solution to Clairaut's equation can be obtained by replacing p in the ODE by the arbitrary constant c_1. Now, considering the second factor in (14.40), we also have

$$\frac{dF}{dp} + x = 0, \tag{14.43}$$

which has the form $G(x, p) = 0$. This relation may be used to eliminate p from (14.39) to give a singular solution.

►*Solve*

$$y = px + p^2. \tag{14.44}$$

From (14.42) the general solution is $y = cx + c^2$. But from (14.43) we also have $2p + x = 0 \Rightarrow p = -x/2$. Substituting this into (14.44) we find the singular solution $x^2 + 4y = 0$. ◄

Solution method. *Write the equation in the form (14.39), then the general solution is given by replacing p by some constant c, as shown in (14.42). Using the relation $dF/dp + x = 0$ to eliminate p from the original equation yields the singular solution.*

14.4 Exercises

14.1 A radioactive isotope decays in such a way that the number of atoms present at a given time, $N(t)$, obeys the equation

$$\frac{dN}{dt} = -\lambda N.$$

If there are initially N_0 atoms present, find $N(t)$ at later times.

14.2 Solve the following equations by separation of the variables:

(a) $y' - xy^3 = 0$;
(b) $y' \tan^{-1} x - y(1 + x^2)^{-1} = 0$;
(c) $x^2 y' + xy^2 = 4y^2$.

14.3 Show that the following equations either are exact or can be made exact, and solve them:

(a) $y(2x^2y^2 + 1)y' + x(y^4 + 1) = 0$;
(b) $2xy' + 3x + y = 0$;
(c) $(\cos^2 x + y \sin 2x)y' + y^2 = 0$.

14.4 Find the values of α and β that make

$$dF(x, y) = \left(\frac{1}{x^2 + 2} + \frac{\alpha}{y}\right) dx + (xy^\beta + 1)\, dy$$

an exact differential. For these values solve $F(x, y) = 0$.

14.5 By finding suitable integrating factors, solve the following equations:

(a) $(1-x^2)y' + 2xy = (1-x^2)^{3/2}$;
(b) $y' - y\cot x + \operatorname{cosec} x = 0$;
(c) $(x+y^3)y' = y$ (treat y as the independent variable).

14.6 By finding an appropriate integrating factor, solve

$$\frac{dy}{dx} = -\frac{2x^2 + y^2 + x}{xy}.$$

14.7 Find, in the form of an integral, the solution of the equation

$$\alpha\frac{dy}{dt} + y = f(t)$$

for a general function $f(t)$. Find the specific solutions for

(a) $f(t) = H(t)$,
(b) $f(t) = \delta(t)$,
(c) $f(t) = \beta^{-1}e^{-t/\beta}H(t)$ with $\beta < \alpha$.

For case (c), what happens if $\beta \to 0$?

14.8 A series electric circuit contains a resistance R, a capacitance C and a battery supplying a time-varying electromotive force $V(t)$. The charge q on the capacitor therefore obeys the equation

$$R\frac{dq}{dt} + \frac{q}{C} = V(t).$$

Assuming that initially there is no charge on the capacitor, and given that $V(t) = V_0 \sin\omega t$, find the charge on the capacitor as a function of time.

14.9 Using tangential–polar coordinates (see exercise 2.20), consider a particle of mass m moving under the influence of a force f directed towards the origin O. By resolving forces along the instantaneous tangent and normal and making use of the result of exercise 2.20 for the instantaneous radius of curvature, prove that

$$f = -mv\frac{dv}{dr} \qquad \text{and} \qquad mv^2 = fp\frac{dr}{dp}.$$

Show further that $h = mpv$ is a constant of the motion and that the law of force can be deduced from

$$f = \frac{h^2}{mp^3}\frac{dp}{dr}.$$

14.10 Use the result of exercise 14.9 to find the law of force, acting towards the origin, under which a particle must move so as to describe the following trajectories:

(a) A circle of radius a that passes through the origin;
(b) An equiangular spiral, which is defined by the property that the angle α between the tangent and the radius vector is constant along the curve.

14.11 Solve

$$(y-x)\frac{dy}{dx} + 2x + 3y = 0.$$

14.12 A mass m is accelerated by a time-varying force $\alpha\exp(-\beta t)v^3$, where v is its velocity. It also experiences a resistive force ηv, where η is a constant, owing to its motion through the air. The equation of motion of the mass is therefore

$$m\frac{dv}{dt} = \alpha\exp(-\beta t)v^3 - \eta v.$$

Find an expression for the velocity v of the mass as a function of time, given that it has an initial velocity v_0.

14.13 Using the results about Laplace transforms given in chapter 13 for df/dt and $tf(t)$, show, for a function $y(t)$ that satisfies

$$t\frac{dy}{dt} + (t-1)y = 0 \qquad (*)$$

with $y(0)$ finite, that $\bar{y}(s) = C(1+s)^{-2}$ for some constant C.

Given that

$$y(t) = t + \sum_{n=2}^{\infty} a_n t^n,$$

determine C and show that $a_n = (-1)^{n-1}/(n-1)!$. Compare this result with that obtained by integrating $(*)$ directly.

14.14 Solve

$$\frac{dy}{dx} = \frac{1}{x+2y+1}.$$

14.15 Solve

$$\frac{dy}{dx} = -\frac{x+y}{3x+3y-4}.$$

14.16 If $u = 1 + \tan y$, calculate $d(\ln u)/dy$; hence find the general solution of

$$\frac{dy}{dx} = \tan x \cos y\ (\cos y + \sin y).$$

14.17 Solve

$$x(1-2x^2y)\frac{dy}{dx} + y = 3x^2y^2,$$

given that $y(1) = 1/2$.

14.18 A reflecting mirror is made in the shape of the surface of revolution generated by revolving the curve $y(x)$ about the x-axis. In order that light rays emitted from a point source at the origin are reflected back parallel to the x-axis, the curve $y(x)$ must obey

$$\frac{y}{x} = \frac{2p}{1-p^2},$$

where $p = dy/dx$. By solving this equation for x, find the curve $y(x)$.

14.19 Find the curve with the property that at each point on it the sum of the intercepts on the x- and y-axes of the tangent to the curve (taking account of sign) is equal to 1.

14.20 Find a parametric solution of

$$x\left(\frac{dy}{dx}\right)^2 + \frac{dy}{dx} - y = 0$$

as follows.

(a) Write an equation for y in terms of $p = dy/dx$ and show that

$$p = p^2 + (2px+1)\frac{dp}{dx}.$$

(b) Using p as the independent variable, arrange this as a linear first-order equation for x.

(c) Find an appropriate integrating factor to obtain

$$x = \frac{\ln p - p + c}{(1-p)^2},$$

which, together with the expression for y obtained in (a), gives a parameterisation of the solution.

(d) Reverse the roles of x and y in steps (a) to (c), putting $dx/dy = p^{-1}$, and show that essentially the same parameterisation is obtained.

14.21 Using the substitutions $u = x^2$ and $v = y^2$, reduce the equation

$$xy\left(\frac{dy}{dx}\right)^2 - (x^2 + y^2 - 1)\frac{dy}{dx} + xy = 0$$

to Clairaut's form. Hence show that the equation represents a family of conics and the four sides of a square.

14.22 The action of the control mechanism on a particular system for an input $f(t)$ is described, for $t \geq 0$, by the coupled first-order equations:

$$\dot{y} + 4z = f(t),$$
$$\dot{z} - 2z = \dot{y} + \tfrac{1}{2}y.$$

Use Laplace transforms to find the response $y(t)$ of the system to a unit step input, $f(t) = H(t)$, given that $y(0) = 1$ and $z(0) = 0$.

Questions 23 to 31 are intended to give the reader practice in choosing an appropriate method. The level of difficulty varies within the set; if necessary, the hints may be consulted for an indication of the most appropriate approach.

14.23 Find the general solutions of the following:

(a) $\dfrac{dy}{dx} + \dfrac{xy}{a^2 + x^2} = x$; (b) $\dfrac{dy}{dx} = \dfrac{4y^2}{x^2} - y^2$.

14.24 Solve the following first-order equations for the boundary conditions given:

(a) $y' - (y/x) = 1$, $y(1) = -1$;
(b) $y' - y\tan x = 1$, $y(\pi/4) = 3$;
(c) $y' - y^2/x^2 = 1/4$, $y(1) = 1$;
(d) $y' - y^2/x^2 = 1/4$, $y(1) = 1/2$.

14.25 An electronic system has two inputs, to each of which a constant unit signal is applied, but starting at different times. The equations governing the system thus take the form

$$\dot{x} + 2y = H(t),$$
$$\dot{y} - 2x = H(t-3).$$

Initially (at $t = 0$), $x = 1$ and $y = 0$; find $x(t)$ at later times.

14.26 Solve the differential equation

$$\sin x\frac{dy}{dx} + 2y\cos x = 1,$$

subject to the boundary condition $y(\pi/2) = 1$.

14.27 Find the complete solution of

$$\left(\frac{dy}{dx}\right)^2 - \frac{y}{x}\frac{dy}{dx} + \frac{A}{x} = 0,$$

where A is a positive constant.

14.28 Find the solution of

$$(5x + y - 7)\frac{dy}{dx} = 3(x + y + 1).$$

14.29 Find the solution $y = y(x)$ of

$$x\frac{dy}{dx} + y - \frac{y^2}{x^{3/2}} = 0,$$

subject to $y(1) = 1$.

14.30 Find the solution of

$$(2\sin y - x)\frac{dy}{dx} = \tan y,$$

if (a) $y(0) = 0$, and (b) $y(0) = \pi/2$.

14.31 Find the family of solutions of

$$\frac{d^2y}{dx^2} + \left(\frac{dy}{dx}\right)^2 + \frac{dy}{dx} = 0$$

that satisfy $y(0) = 0$.

14.5 Hints and answers

14.1 $N(t) = N_0 \exp(-\lambda t)$.

14.3 (a) exact, $x^2y^4 + x^2 + y^2 = c$; (b) IF $= x^{-1/2}$, $x^{1/2}(x + y) = c$; (c) IF $= \sec^2 x$, $y^2 \tan x + y = c$.

14.5 (a) IF $= (1 - x^2)^{-2}$, $y = (1 - x^2)(k + \sin^{-1} x)$; (b) IF $= \operatorname{cosec} x$, leading to $y = k\sin x + \cos x$; (c) exact equation is $y^{-1}(dx/dy) - xy^{-2} = y$, leading to $x = y(k + y^2/2)$.

14.7 $y(t) = e^{-t/\alpha}\int^t \alpha^{-1}e^{t'/\alpha}f(t')dt'$; (a) $y(t) = 1 - e^{-t/\alpha}$; (b) $y(t) = \alpha^{-1}e^{-t/\alpha}$; (c) $y(t) = (e^{-t/\alpha} - e^{-t/\beta})/(\alpha - \beta)$. It becomes case (b).

14.9 Note that, if the angle between the tangent and the radius vector is α, then $\cos\alpha = dr/ds$ and $\sin\alpha = p/r$.

14.11 Homogeneous equation, put $y = vx$ to obtain $(1 - v)(v^2 + 2v + 2)^{-1}\,dv = x^{-1}\,dx$; write $1 - v$ as $2 - (1 + v)$, and $v^2 + 2v + 2$ as $1 + (1 + v)^2$; $A[x^2 + (x + y)^2] = \exp\left\{4\tan^{-1}[(x + y)/x]\right\}$.

14.13 $(1 + s)(d\bar{y}/ds) + 2\bar{y} = 0$. $C = 1$; use separation of variables to show directly that $y(t) = te^{-t}$.

14.15 The equation is of the form of (14.22), set $v = x + y$; $x + 3y + 2\ln(x + y - 2) = A$.

14.17 The equation is isobaric with weight $y = -2$; setting $y = vx^{-2}$ gives $v^{-1}(1 - v)^{-1}(1 - 2v)\,dv = x^{-1}\,dx$; $4xy(1 - x^2y) = 1$.

14.19 The curve must satisfy $y = (1 - p^{-1})^{-1}(1 - x + px)$, which has solution $x = (p - 1)^{-2}$, leading to $y = (1 \pm \sqrt{x})^2$ or $x = (1 \pm \sqrt{y})^2$; the singular solution $p' = 0$ gives straight lines joining $(\theta, 0)$ and $(0, 1 - \theta)$ for any θ.

14.21 $v = qu + q/(q - 1)$, where $q = dv/du$. General solution $y^2 = cx^2 + c/(c - 1)$, hyperbolae for $c > 0$ and ellipses for $c < 0$. Singular solution $y = \pm(x \pm 1)$.

14.23 (a) Integrating factor is $(a^2 + x^2)^{1/2}$, $y = (a^2 + x^2)/3 + A(a^2 + x^2)^{-1/2}$; (b) separable, $y = x(x^2 + Ax + 4)^{-1}$.

14.25 Use Laplace transforms; $\bar{x}s(s^2 + 4) = s + s^2 - 2e^{-3s}$; $x(t) = \frac{1}{2}\sin 2t + \cos 2t - \frac{1}{2}H(t - 3) + \frac{1}{2}\cos(2t - 6)H(t - 3)$.

14.27 This is Clairaut's equation with $F(p) = A/p$. General solution $y = cx + A/c$; singular solution, $y = 2\sqrt{Ax}$.

14.29 Either Bernoulli's equation with $n = 2$ or an isobaric equation with $m = 3/2$; $y(x) = 5x^{3/2}/(2 + 3x^{5/2})$.

14.31 Show that $p = (Ce^x - 1)^{-1}$, where $p = dy/dx$; $y = \ln[C - e^{-x})/(C - 1)]$ or $\ln[D - (D - 1)e^{-x}]$ or $\ln(e^{-K} + 1 - e^{-x}) + K$.

15

Higher-order ordinary differential equations

Following on from the discussion of first-order ordinary differential equations (ODEs) given in the previous chapter, we now examine equations of second and higher order. Since a brief outline of the general properties of ODEs and their solutions was given at the beginning of the previous chapter, we will not repeat it here. Instead, we will begin with a discussion of various types of higher-order equation. This chapter is divided into three main parts. We first discuss linear equations with constant coefficients and then investigate linear equations with variable coefficients. Finally, we discuss a few methods that may be of use in solving general linear or non-linear ODEs. Let us start by considering some general points relating to *all* linear ODEs.

Linear equations are of paramount importance in the description of physical processes. Moreover, it is an empirical fact that, when put into mathematical form, many natural processes appear as higher-order linear ODEs, most often as second-order equations. Although we could restrict our attention to these second-order equations, the generalisation to nth-order equations requires little extra work, and so we will consider this more general case.

A linear ODE of general order n has the form

$$a_n(x)\frac{d^n y}{dx^n} + a_{n-1}(x)\frac{d^{n-1} y}{dx^{n-1}} + \cdots + a_1(x)\frac{dy}{dx} + a_0(x)y = f(x). \qquad (15.1)$$

If $f(x) = 0$ then the equation is called *homogeneous*; otherwise it is *inhomogeneous*. The first-order linear equation studied in subsection 14.2.4 is a special case of (15.1). As discussed at the beginning of the previous chapter, the general solution to (15.1) will contain n arbitrary constants, which may be determined if n boundary conditions are also provided.

In order to solve any equation of the form (15.1), we must first find the general solution of the *complementary equation*, i.e. the equation formed by setting

$f(x) = 0$:

$$a_n(x)\frac{d^n y}{dx^n} + a_{n-1}(x)\frac{d^{n-1}y}{dx^{n-1}} + \cdots + a_1(x)\frac{dy}{dx} + a_0(x)y = 0. \tag{15.2}$$

To determine the general solution of (15.2), we must find n linearly independent functions that satisfy it. Once we have found these solutions, the general solution is given by a linear superposition of these n functions. In other words, if the n solutions of (15.2) are $y_1(x)$, $y_2(x), \ldots, y_n(x)$, then the general solution is given by the linear superposition

$$y_c(x) = c_1 y_1(x) + c_2 y_2(x) + \cdots + c_n y_n(x), \tag{15.3}$$

where the c_m are arbitrary constants that may be determined if n boundary conditions are provided. The linear combination $y_c(x)$ is called the *complementary function* of (15.1).

The question naturally arises how we establish that any n individual solutions to (15.2) are indeed linearly independent. For n functions to be linearly independent over an interval, there must not exist *any* set of constants c_1, $c_2, \ldots, c_n$ such that

$$c_1 y_1(x) + c_2 y_2(x) + \cdots + c_n y_n(x) = 0 \tag{15.4}$$

over the interval in question, except for the trivial case $c_1 = c_2 = \cdots = c_n = 0$.

A statement equivalent to (15.4), which is perhaps more useful for the practical determination of linear independence, can be found by repeatedly differentiating (15.4), $n-1$ times in all, to obtain n simultaneous equations for c_1, $c_2, \ldots, c_n$:

$$\begin{aligned} c_1 y_1(x) + c_2 y_2(x) + \cdots + c_n y_n(x) &= 0 \\ c_1 y_1'(x) + c_2 y_2'(x) + \cdots + c_n y_n'(x) &= 0 \\ &\vdots \\ c_1 y_1^{(n-1)}(x) + c_2 y_2^{(n-1)} + \cdots + c_n y_n^{(n-1)}(x) &= 0, \end{aligned} \tag{15.5}$$

where the primes denote differentiation with respect to x. Referring to the discussion of simultaneous linear equations given in chapter 8, if the determinant of the coefficients of c_1, $c_2, \ldots, c_n$ is non-zero then the only solution to equations (15.5) is the trivial solution $c_1 = c_2 = \cdots = c_n = 0$. In other words, the n functions $y_1(x)$, $y_2(x), \ldots, y_n(x)$ are linearly independent over an interval if

$$W(y_1, y_2, \ldots, y_n) = \begin{vmatrix} y_1 & y_2 & \ldots & y_n \\ y_1' & y_2' & & \vdots \\ \vdots & & \ddots & \vdots \\ y_1^{(n-1)} & \ldots & \ldots & y_n^{(n-1)} \end{vmatrix} \neq 0 \tag{15.6}$$

over that interval; $W(y_1, y_2, \ldots, y_n)$ is called the *Wronskian* of the set of functions. It should be noted, however, that the vanishing of the Wronskian does not guarantee that the functions are linearly dependent.

If the original equation (15.1) has $f(x) = 0$ (i.e. it is homogeneous) then of course the complementary function $y_c(x)$ in (15.3) is already the general solution. If, however, the equation has $f(x) \neq 0$ (i.e. it is inhomogeneous) then $y_c(x)$ is only one part of the solution. The general solution of (15.1) is then given by

$$y(x) = y_c(x) + y_p(x), \tag{15.7}$$

where $y_p(x)$ is the *particular integral*, which can be *any* function that satisfies (15.1) directly, provided it is linearly independent of $y_c(x)$. It should be emphasised for practical purposes that *any* such function, no matter how simple (or complicated), is equally valid in forming the general solution (15.7).

It is important to realise that the above method for finding the general solution to an ODE by superposing particular solutions assumes crucially that the ODE is linear. For non-linear equations, discussed in section 15.3, this method cannot be used, and indeed it is often impossible to find closed-form solutions to such equations.

15.1 Linear equations with constant coefficients

If the a_m in (15.1) are constants rather than functions of x then we have

$$a_n \frac{d^n y}{dx^n} + a_{n-1} \frac{d^{n-1} y}{dx^{n-1}} + \cdots + a_1 \frac{dy}{dx} + a_0 y = f(x). \tag{15.8}$$

Equations of this sort are very common throughout the physical sciences and engineering, and the method for their solution falls into two parts as discussed in the previous section, i.e. finding the complementary function $y_c(x)$ and finding the particular integral $y_p(x)$. If $f(x) = 0$ in (15.8) then we do not have to find a particular integral, and the complementary function is by itself the general solution.

15.1.1 Finding the complementary function $y_c(x)$

The complementary function must satisfy

$$a_n \frac{d^n y}{dx^n} + a_{n-1} \frac{d^{n-1} y}{dx^{n-1}} + \cdots + a_1 \frac{dy}{dx} + a_0 y = 0 \tag{15.9}$$

and contain n arbitrary constants (see equation (15.3)). The standard method for finding $y_c(x)$ is to try a solution of the form $y = Ae^{\lambda x}$, substituting this into (15.9). After dividing the resulting equation through by $Ae^{\lambda x}$, we are left with a polynomial equation in λ of order n; this is the *auxiliary equation* and reads

$$a_n \lambda^n + a_{n-1} \lambda^{n-1} + \cdots + a_1 \lambda + a_0 = 0. \tag{15.10}$$

In general the auxiliary equation has n roots, say $\lambda_1, \lambda_2, \ldots, \lambda_n$. In certain cases, some of these roots may be repeated and some may be complex. The three main cases are as follows.

(i) *All roots real and distinct.* In this case the n solutions to (15.9) are $\exp \lambda_m x$ for $m = 1$ to n. It is easily shown by calculating the Wronskian (15.6) of these functions that if all the λ_m are distinct then these solutions are linearly independent. We can therefore linearly superpose them, as in (15.3), to form the complementary function

$$y_c(x) = c_1 e^{\lambda_1 x} + c_2 e^{\lambda_2 x} + \cdots + c_n e^{\lambda_n x}. \tag{15.11}$$

(ii) *Some roots complex.* For the special (but usual) case that all the coefficients a_m in (15.9) are real, if one of the roots of the auxiliary equation (15.10) is complex, say $\alpha + i\beta$, then its complex conjugate $\alpha - i\beta$ is also a root. In this case we can write

$$\begin{aligned} c_1 e^{(\alpha+i\beta)x} + c_2 e^{(\alpha-i\beta)x} &= e^{\alpha x}(d_1 \cos \beta x + d_2 \sin \beta x) \\ &= A e^{\alpha x} \left\{ \begin{array}{c} \sin \\ \cos \end{array} \right\} (\beta x + \phi), \end{aligned} \tag{15.12}$$

where A and ϕ are arbitrary constants.

(iii) *Some roots repeated.* If, for example, λ_1 occurs k times ($k > 1$) as a root of the auxiliary equation, then we have not found n linearly independent solutions of (15.9); formally the Wronskian (15.6) of these solutions, having two or more identical columns, is equal to zero. We must therefore find $k-1$ further solutions that are linearly independent of those already found and also of each other. By direct substitution into (15.9) we find that

$$xe^{\lambda_1 x}, \quad x^2 e^{\lambda_1 x}, \quad \ldots, \quad x^{k-1} e^{\lambda_1 x}$$

are also solutions, and by calculating the Wronskian it is easily shown that they, together with the solutions already found, form a linearly independent set of n functions. Therefore the complementary function is given by

$$y_c(x) = (c_1 + c_2 x + \cdots + c_k x^{k-1}) e^{\lambda_1 x} + c_{k+1} e^{\lambda_{k+1} x} + c_{k+2} e^{\lambda_{k+2} x} + \cdots + c_n e^{\lambda_n x}. \tag{15.13}$$

If more than one root is repeated the above argument is easily extended. For example, suppose as before that λ_1 is a k-fold root of the auxiliary equation and, further, that λ_2 is an l-fold root (of course, $k > 1$ and $l > 1$). Then, from the above argument, the complementary function reads

$$\begin{aligned} y_c(x) = {} & (c_1 + c_2 x + \cdots + c_k x^{k-1}) e^{\lambda_1 x} \\ & + (c_{k+1} + c_{k+2} x + \cdots + c_{k+l} x^{l-1}) e^{\lambda_2 x} \\ & + c_{k+l+1} e^{\lambda_{k+l+1} x} + c_{k+l+2} e^{\lambda_{k+l+2} x} + \cdots + c_n e^{\lambda_n x}. \end{aligned} \tag{15.14}$$

►*Find the complementary function of the equation*

$$\frac{d^2y}{dx^2} - 2\frac{dy}{dx} + y = e^x. \tag{15.15}$$

Setting the RHS to zero, substituting $y = Ae^{\lambda x}$ and dividing through by $Ae^{\lambda x}$ we obtain the auxiliary equation

$$\lambda^2 - 2\lambda + 1 = 0.$$

The root $\lambda = 1$ occurs twice and so, although e^x is a solution to (15.15), we must find a further solution to the equation that is linearly independent of e^x. From the above discussion, we deduce that xe^x is such a solution, so that the full complementary function is given by the linear superposition

$$y_c(x) = (c_1 + c_2x)e^x. \blacktriangleleft$$

Solution method. *Set the RHS of the ODE to zero (if it is not already so), and substitute $y = Ae^{\lambda x}$. After dividing through the resulting equation by $Ae^{\lambda x}$, obtain an nth-order polynomial equation in λ (the auxiliary equation, see (15.10)). Solve the auxiliary equation to find the n roots, $\lambda_1, \lambda_2, \ldots, \lambda_n$, say. If all these roots are real and distinct then $y_c(x)$ is given by (15.11). If, however, some of the roots are complex or repeated then $y_c(x)$ is given by (15.12) or (15.13), or the extension (15.14) of the latter, respectively.*

15.1.2 Finding the particular integral $y_p(x)$

There is no generally applicable method for finding the particular integral $y_p(x)$ but, for linear ODEs with constant coefficients and a simple RHS, $y_p(x)$ can often be found by inspection or by assuming a parameterised form similar to $f(x)$. The latter method is sometimes called the *method of undetermined coefficients*. If $f(x)$ contains only polynomial, exponential, or sine and cosine terms then, by assuming a trial function for $y_p(x)$ of similar form but one which contains a number of undetermined parameters and substituting this trial function into (15.9), the parameters can be found and $y_p(x)$ deduced. Standard trial functions are as follows.

(i) If $f(x) = ae^{rx}$ then try

$$y_p(x) = be^{rx}.$$

(ii) If $f(x) = a_1 \sin rx + a_2 \cos rx$ (a_1 or a_2 may be zero) then try

$$y_p(x) = b_1 \sin rx + b_2 \cos rx.$$

(iii) If $f(x) = a_0 + a_1x + \cdots + a_Nx^N$ (some a_m may be zero) then try

$$y_p(x) = b_0 + b_1x + \cdots + b_Nx^N.$$

(iv) If $f(x)$ is the sum or product of any of the above then try $y_p(x)$ as the sum or product of the corresponding individual trial functions.

It should be noted that this method fails if any term in the assumed trial function is also contained within the complementary function $y_c(x)$. In such a case the trial function should be multiplied by the smallest integer power of x such that it will then contain no term that already appears in the complementary function. The undetermined coefficients in the trial function can now be found by substitution into (15.8).

Three further methods that are useful in finding the particular integral $y_p(x)$ are those based on Green's functions, the variation of parameters, and a change in the dependent variable using knowledge of the complementary function. However, since these methods are also applicable to equations with variable coefficients, a discussion of them is postponed until section 15.2.

►*Find a particular integral of the equation*

$$\frac{d^2y}{dx^2} - 2\frac{dy}{dx} + y = e^x.$$

From the above discussion our first guess at a trial particular integral would be $y_p(x) = be^x$. However, since the complementary function of this equation is $y_c(x) = (c_1 + c_2x)e^x$ (as in the previous subsection), we see that e^x is already contained in it, as indeed is xe^x. Multiplying our first guess by the lowest integer power of x such that the result does not appear in $y_c(x)$, we therefore try $y_p(x) = bx^2e^x$. Substituting this into the ODE, we find that $b = 1/2$, so the particular integral is given by $y_p(x) = x^2e^x/2$. ◄

Solution method. *If the RHS of an ODE contains only functions mentioned at the start of this subsection then the appropriate trial function should be substituted into it, thereby fixing the undetermined parameters. If, however, the RHS of the equation is not of this form then one of the more general methods outlined in subsections 15.2.3–15.2.5 should be used; perhaps the most straightforward of these is the variation-of-parameters method.*

15.1.3 Constructing the general solution $y_c(x) + y_p(x)$

As stated earlier, the full solution to the ODE (15.8) is found by adding together the complementary function and any particular integral. In order to illustrate further the material discussed in the last two subsections, let us find the general solution to a new example, starting from the beginning.

►*Solve*

$$\frac{d^2y}{dx^2} + 4y = x^2 \sin 2x. \tag{15.16}$$

First we set the RHS to zero and assume the trial solution $y = Ae^{\lambda x}$. Substituting this into (15.16) leads to the auxiliary equation

$$\lambda^2 + 4 = 0 \qquad \Rightarrow \qquad \lambda = \pm 2i. \tag{15.17}$$

Therefore the complementary function is given by

$$y_c(x) = c_1 e^{2ix} + c_2 e^{-2ix} = d_1 \cos 2x + d_2 \sin 2x. \tag{15.18}$$

We must now turn our attention to the particular integral $y_p(x)$. Consulting the list of standard trial functions in the previous subsection, we find that a first guess at a suitable trial function for this case should be

$$(ax^2 + bx + c)\sin 2x + (dx^2 + ex + f)\cos 2x. \tag{15.19}$$

However, we see that this trial function contains terms in $\sin 2x$ and $\cos 2x$, both of which already appear in the complementary function (15.18). We must therefore multiply (15.19) by the smallest integer power of x which ensures that none of the resulting terms appears in $y_c(x)$. Since multiplying by x will suffice, we finally assume the trial function

$$(ax^3 + bx^2 + cx)\sin 2x + (dx^3 + ex^2 + fx)\cos 2x. \tag{15.20}$$

Substituting this into (15.16) to fix the constants appearing in (15.20), we find the particular integral to be

$$y_p(x) = -\frac{x^3}{12}\cos 2x + \frac{x^2}{16}\sin 2x + \frac{x}{32}\cos 2x. \tag{15.21}$$

The general solution to (15.16) then reads

$$\begin{aligned} y(x) &= y_c(x) + y_p(x) \\ &= d_1 \cos 2x + d_2 \sin 2x - \frac{x^3}{12}\cos 2x + \frac{x^2}{16}\sin 2x + \frac{x}{32}\cos 2x. \end{aligned}$$ ◄

15.1.4 Linear recurrence relations

Before continuing our discussion of higher-order ODEs, we take this opportunity to introduce the discrete analogues of differential equations, which are called *recurrence relations* (or sometimes *difference equations*). Whereas a differential equation gives a prescription, in terms of current values, for the new value of a dependent variable at a point only infinitesimally far away, a recurrence relation describes how the next in a sequence of values u_n, defined only at (non-negative) integer values of the 'independent variable' n, is to be calculated.

In its most general form a recurrence relation expresses the way in which u_{n+1} is to be calculated from all the preceding values $u_0, u_1, \ldots, u_n$. Just as the most general differential equations are intractable, so are the most general recurrence relations, and we will limit ourselves to analogues of the types of differential equations studied earlier in this chapter, namely those that are linear, have constant coefficients and possess simple functions on the RHS. Such equations occur over a broad range of engineering and statistical physics as well as in the realms of finance, business planning and gambling! They form the basis of many numerical methods, particularly those concerned with the numerical solution of ordinary and partial differential equations.

A general recurrence relation is exemplified by the formula

$$u_{n+1} = \sum_{r=0}^{N-1} a_r u_{n-r} + k, \tag{15.22}$$

where N and the a_r are fixed and k is a constant or a simple function of n. Such an equation, involving terms of the series whose indices differ by up to N (ranging from $n-N+1$ to n), is called an Nth-order recurrence relation. It is clear that, given values for $u_0, u_1, \ldots, u_{N-1}$, this is a definitive scheme for generating the series and therefore has a unique solution.

Parallelling the nomenclature of differential equations, if the term not involving any u_n is absent, i.e. $k = 0$, then the recurrence relation is called *homogeneous*. The parallel continues with the form of the general solution of (15.22). If v_n is the general solution of the homogeneous relation, and w_n is *any* solution of the full relation, then

$$u_n = v_n + w_n$$

is the most general solution of the complete recurrence relation. This is straightforwardly verified as follows:

$$\begin{aligned} u_{n+1} &= v_{n+1} + w_{n+1} \\ &= \sum_{r=0}^{N-1} a_r v_{n-r} + \sum_{r=0}^{N-1} a_r w_{n-r} + k \\ &= \sum_{r=0}^{N-1} a_r (v_{n-r} + w_{n-r}) + k \\ &= \sum_{r=0}^{N-1} a_r u_{n-r} + k. \end{aligned}$$

Of course, if $k = 0$ then $w_n = 0$ for all n is a trivial particular solution and the complementary solution, v_n, is itself the most general solution.

First-order recurrence relations

First-order relations, for which $N = 1$, are exemplified by

$$u_{n+1} = au_n + k, \tag{15.23}$$

with u_0 specified. The solution to the homogeneous relation is immediate,

$$u_n = Ca^n,$$

and, if k is a constant, the particular solution is equally straightforward: $w_n = K$ for all n, provided K is chosen to satisfy

$$K = aK + k,$$

i.e. $K = k(1-a)^{-1}$. This will be sufficient unless $a = 1$, in which case $u_n = u_0 + nk$ is obvious by inspection.

Thus the general solution of (15.23) is

$$u_n = \begin{cases} Ca^n + k/(1-a) & a \neq 1, \\ u_0 + nk & a = 1. \end{cases} \tag{15.24}$$

If u_0 is specified for the case of $a \neq 1$ then C must be chosen as $C = u_0 - k/(1-a)$, resulting in the equivalent form

$$u_n = u_0 a^n + k\frac{1-a^n}{1-a}. \tag{15.25}$$

We now illustrate this method with a worked example.

►*A house-buyer borrows capital B from a bank that charges a fixed annual rate of interest R%. If the loan is to be repaid over Y years, at what value should the fixed annual payments P, made at the end of each year, be set? For a loan over 25 years at 6%, what percentage of the first year's payment goes towards paying off the capital?*

Let u_n denote the outstanding debt at the end of year n, and write $R/100 = r$. Then the relevant recurrence relation is

$$u_{n+1} = u_n(1+r) - P$$

with $u_0 = B$. From (15.25) we have

$$u_n = B(1+r)^n - P\frac{1-(1+r)^n}{1-(1+r)}.$$

As the loan is to be repaid over Y years, $u_Y = 0$ and thus

$$P = \frac{Br(1+r)^Y}{(1+r)^Y - 1}.$$

The first year's interest is rB and so the fraction of the first year's payment going towards capital repayment is $(P - rB)/P$, which, using the above expression for P, is equal to $(1+r)^{-Y}$. With the given figures, this is (only) 23%. ◄

With only small modifications, the method just described can be adapted to handle recurrence relations in which the constant k in (15.23) is replaced by $k\alpha^n$, i.e. the relation is

$$u_{n+1} = au_n + k\alpha^n. \tag{15.26}$$

As for an inhomogeneous linear differential equation (see subsection 15.1.2), we may try as a potential particular solution a form which resembles the term that makes the equation inhomogeneous. Here, the presence of the term $k\alpha^n$ indicates that a particular solution of the form $u_n = A\alpha^n$ should be tried. Substituting this into (15.26) gives

$$A\alpha^{n+1} = aA\alpha^n + k\alpha^n,$$

from which it follows that $A = k/(\alpha - a)$ and that there is a particular solution having the form $u_n = k\alpha^n/(\alpha - a)$, provided $\alpha \neq a$. For the special case $\alpha = a$, the reader can readily verify that a particular solution of the form $u_n = An\alpha^n$ is appropriate. This mirrors the corresponding situation for linear differential equations when the RHS of the differential equation is contained in the complementary function of its LHS.

In summary, the general solution to (15.26) is

$$u_n = \begin{cases} C_1 a^n + k\alpha^n/(\alpha - a) & \alpha \neq a, \\ C_2 a^n + kn\alpha^{n-1} & \alpha = a, \end{cases} \tag{15.27}$$

with $C_1 = u_0 - k/(\alpha - a)$ and $C_2 = u_0$.

Second-order recurrence relations

We consider next recurrence relations that involve u_{n-1} in the prescription for u_{n+1} and treat the general case in which the intervening term, u_n, is also present. A typical equation is thus

$$u_{n+1} = au_n + bu_{n-1} + k. \tag{15.28}$$

As previously, the general solution of this is $u_n = v_n + w_n$, where v_n satisfies

$$v_{n+1} = av_n + bv_{n-1} \tag{15.29}$$

and w_n is *any* particular solution of (15.28); the proof follows the same lines as that given earlier.

We have already seen for a first-order recurrence relation that the solution to the homogeneous equation is given by terms forming a geometric series, and we consider a corresponding series of powers in the present case. Setting $v_n = A\lambda^n$ in (15.29) for some λ, as yet undetermined, gives the requirement that λ should satisfy

$$A\lambda^{n+1} = aA\lambda^n + bA\lambda^{n-1}.$$

Dividing through by $A\lambda^{n-1}$ (assumed non-zero) shows that λ could be either of the roots, λ_1 and λ_2, of

$$\lambda^2 - a\lambda - b = 0, \tag{15.30}$$

which is known as the *characteristic equation* of the recurrence relation.

That there are two possible series of terms of the form $A\lambda^n$ is consistent with the fact that two initial values (boundary conditions) have to be provided before the series can be calculated by repeated use of (15.28). These two values are sufficient to determine the appropriate coefficient A for each of the series. Since (15.29) is both linear and homogeneous, and is satisfied by both $v_n = A\lambda_1^n$ and $v_n = B\lambda_2^n$, its general solution is

$$v_n = A\lambda_1^n + B\lambda_2^n.$$

If the coefficients a and b are such that (15.30) has two equal roots, i.e. $a^2 = -4b$, then, as in the analogous case of repeated roots for differential equations (see subsection 15.1.1(iii)), the second term of the general solution is replaced by $Bn\lambda_1^n$ to give

$$v_n = (A + Bn)\lambda_1^n.$$

Finding a particular solution is straightforward if k is a constant: a trivial but adequate solution is $w_n = k(1 - a - b)^{-1}$ for all n. As with first-order equations, particular solutions can be found for other simple forms of k by trying functions similar to k itself. Thus particular solutions for the cases $k = Cn$ and $k = D\alpha^n$ can be found by trying $w_n = E + Fn$ and $w_n = G\alpha^n$ respectively.

►*Find the value of u_{16} if the series u_n satisfies*

$$u_{n+1} + 4u_n + 3u_{n-1} = n$$

for $n \geq 1$, with $u_0 = 1$ and $u_1 = -1$.

We first solve the characteristic equation,

$$\lambda^2 + 4\lambda + 3 = 0,$$

to obtain the roots $\lambda = -1$ and $\lambda = -3$. Thus the complementary function is

$$v_n = A(-1)^n + B(-3)^n.$$

In view of the form of the RHS of the original relation, we try

$$w_n = E + Fn$$

as a particular solution and obtain

$$E + F(n + 1) + 4(E + Fn) + 3[E + F(n - 1)] = n,$$

yielding $F = 1/8$ and $E = 1/32$.

Thus the complete general solution is

$$u_n = A(-1)^n + B(-3)^n + \frac{n}{8} + \frac{1}{32},$$

and now using the given values for u_0 and u_1 determines A as $7/8$ and B as $3/32$. Thus

$$u_n = \frac{1}{32}\left[28(-1)^n + 3(-3)^n + 4n + 1\right].$$

Finally, substituting $n = 16$ gives $u_{16} = 4\,035\,633$, a value the reader may (or may not) wish to verify by repeated application of the initial recurrence relation. ◄

Higher-order recurrence relations

It will be apparent that linear recurrence relations of order $N > 2$ do not present any additional difficulty in principle, though two obvious practical difficulties are (i) that the characteristic equation is of order N and in general will not have roots that can be written in closed form and (ii) that a correspondingly large number of given values is required to determine the N otherwise arbitrary constants in the solution. The algebraic labour needed to solve the set of simultaneous linear equations that determines them increases rapidly with N. We do not give specific examples here, but some are included in the exercises at the end of the chapter.

15.1.5 Laplace transform method

Having briefly discussed recurrence relations, we now return to the main topic of this chapter, i.e. methods for obtaining solutions to higher-order ODEs. One such method is that of Laplace transforms, which is very useful for solving linear ODEs with constant coefficients. Taking the Laplace transform of such an equation transforms it into a purely *algebraic* equation in terms of the Laplace transform of the required solution. Once the algebraic equation has been solved for this Laplace transform, the general solution to the original ODE can be obtained by performing an inverse Laplace transform. One advantage of this method is that, for given boundary conditions, it provides the solution in just one step, instead of having to find the complementary function and particular integral separately.

In order to apply the method we need only two results from Laplace transform theory (see section 13.2). First, the Laplace transform of a function $f(x)$ is defined by

$$\bar{f}(s) \equiv \int_0^\infty e^{-sx} f(x)\, dx, \tag{15.31}$$

from which we can derive the second useful relation. This concerns the Laplace transform of the nth derivative of $f(x)$:

$$\overline{f^{(n)}}(s) = s^n \bar{f}(s) - s^{n-1} f(0) - s^{n-2} f'(0) - \cdots - s f^{(n-2)}(0) - f^{(n-1)}(0), \tag{15.32}$$

where the primes and superscripts in parentheses denote differentiation with respect to x. Using these relations, along with table 13.1, on p. 455, which gives Laplace transforms of standard functions, we are in a position to solve a linear ODE with constant coefficients by this method.

►*Solve*

$$\frac{d^2y}{dx^2} - 3\frac{dy}{dx} + 2y = 2e^{-x}, \tag{15.33}$$

subject to the boundary conditions $y(0) = 2$, $y'(0) = 1$.

Taking the Laplace transform of (15.33) and using the table of standard results we obtain

$$s^2\bar{y}(s) - sy(0) - y'(0) - 3\left[s\bar{y}(s) - y(0)\right] + 2\bar{y}(s) = \frac{2}{s+1},$$

which reduces to

$$(s^2 - 3s + 2)\bar{y}(s) - 2s + 5 = \frac{2}{s+1}. \tag{15.34}$$

Solving this algebraic equation for $\bar{y}(s)$, the Laplace transform of the required solution to (15.33), we obtain

$$\bar{y}(s) = \frac{2s^2 - 3s - 3}{(s+1)(s-1)(s-2)} = \frac{1}{3(s+1)} + \frac{2}{s-1} - \frac{1}{3(s-2)}, \tag{15.35}$$

where in the final step we have used partial fractions. Taking the inverse Laplace transform of (15.35), again using table 13.1, we find the specific solution to (15.33) to be

$$y(x) = \tfrac{1}{3}e^{-x} + 2e^{x} - \tfrac{1}{3}e^{2x}. \blacktriangleleft$$

Note that if the boundary conditions in a problem are given as symbols, rather than just numbers, then the step involving partial fractions can often involve a considerable amount of algebra. The Laplace transform method is also very convenient for solving sets of *simultaneous* linear ODEs with constant coefficients.

►*Two electrical circuits, both of negligible resistance, each consist of a coil having self-inductance* L *and a capacitor having capacitance* C. *The mutual inductance of the two circuits is* M. *There is no source of e.m.f. in either circuit. Initially the second capacitor is given a charge* CV_0, *the first capacitor being uncharged, and at time* $t = 0$ *a switch in the second circuit is closed to complete the circuit. Find the subsequent current in the first circuit.*

Subject to the initial conditions $q_1(0) = \dot{q}_1(0) = \dot{q}_2(0) = 0$ and $q_2(0) = CV_0 = V_0/G$, say, we have to solve

$$L\ddot{q}_1 + M\ddot{q}_2 + Gq_1 = 0,$$
$$M\ddot{q}_1 + L\ddot{q}_2 + Gq_2 = 0.$$

On taking the Laplace transform of the above equations, we obtain

$$(Ls^2 + G)\bar{q}_1 + Ms^2\bar{q}_2 = sMV_0C,$$
$$Ms^2\bar{q}_1 + (Ls^2 + G)\bar{q}_2 = sLV_0C.$$

Eliminating $\bar{q}_2$ and rewriting as an equation for $\bar{q}_1$, we find

$$\bar{q}_1(s) = \frac{MV_0 s}{[(L+M)s^2 + G][(L-M)s^2 + G]}$$
$$= \frac{V_0}{2G}\left[\frac{(L+M)s}{(L+M)s^2 + G} - \frac{(L-M)s}{(L-M)s^2 + G}\right].$$

Using table 13.1,

$$q_1(t) = \tfrac{1}{2}V_0C(\cos\omega_1 t - \cos\omega_2 t),$$

where $\omega_1^2(L+M) = G$ and $\omega_2^2(L-M) = G$. Thus the current is given by

$$i_1(t) = \tfrac{1}{2}V_0C(\omega_2 \sin\omega_2 t - \omega_1 \sin\omega_1 t). \blacktriangleleft$$

Solution method. *Perform a Laplace transform, as defined in (15.31), on the entire equation, using (15.32) to calculate the transform of the derivatives. Then solve the resulting algebraic equation for $\bar{y}(s)$, the Laplace transform of the required solution to the ODE. By using the method of partial fractions and consulting a table of Laplace transforms of standard functions, calculate the inverse Laplace transform. The resulting function $y(x)$ is the solution of the ODE that obeys the given boundary conditions.*

15.2 Linear equations with variable coefficients

There is no generally applicable method of solving equations with coefficients that are functions of x. Nevertheless, there are certain cases in which a solution is possible. Some of the methods discussed in this section are also useful in finding the general solution or particular integral for equations with constant coefficients that have proved impenetrable by the techniques discussed above.

15.2.1 The Legendre and Euler linear equations

Legendre's linear equation has the form

$$a_n(\alpha x+\beta)^n\frac{d^ny}{dx^n} + \cdots + a_1(\alpha x+\beta)\frac{dy}{dx} + a_0 y = f(x), \tag{15.36}$$

where α, β and the a_n are constants and may be solved by making the substitution $\alpha x+\beta = e^t$. We then have

$$\frac{dy}{dx} = \frac{dt}{dx}\frac{dy}{dt} = \frac{\alpha}{\alpha x+\beta}\frac{dy}{dt}$$

$$\frac{d^2y}{dx^2} = \frac{d}{dx}\frac{dy}{dx} = \frac{\alpha^2}{(\alpha x+\beta)^2}\left(\frac{d^2y}{dt^2} - \frac{dy}{dt}\right)$$

and so on for higher derivatives. Therefore we can write the terms of (15.36) as

$$\begin{aligned}
(\alpha x+\beta)\frac{dy}{dx} &= \alpha\frac{dy}{dt},\\
(\alpha x+\beta)^2\frac{d^2y}{dx^2} &= \alpha^2\frac{d}{dt}\left(\frac{d}{dt}-1\right)y,\\
&\ \ \vdots\\
(\alpha x+\beta)^n\frac{d^ny}{dx^n} &= \alpha^n\frac{d}{dt}\left(\frac{d}{dt}-1\right)\cdots\left(\frac{d}{dt}-n+1\right)y.
\end{aligned} \tag{15.37}$$

Substituting equations (15.37) into the original equation (15.36), the latter becomes a linear ODE with constant coefficients, i.e.

$$a_n\alpha^n\frac{d}{dt}\left(\frac{d}{dt}-1\right)\cdots\left(\frac{d}{dt}-n+1\right)y+\cdots+a_1\alpha\frac{dy}{dt}+a_0y=f\left(\frac{e^t-\beta}{\alpha}\right),$$

which can be solved by the methods of section 15.1.

A special case of Legendre's linear equation, for which $\alpha = 1$ and $\beta = 0$, is *Euler's equation*,

$$a_nx^n\frac{d^ny}{dx^n}+\cdots+a_1x\frac{dy}{dx}+a_0y=f(x); \qquad (15.38)$$

it may be solved in a similar manner to the above by substituting $x = e^t$. If $f(x) = 0$ in (15.38) then substituting $y = x^\lambda$ leads to a simple algebraic equation in λ, which can be solved to yield the solution to (15.38). In the event that the algebraic equation for λ has repeated roots, extra care is needed. If λ_1 is a k-fold root ($k > 1$) then the k linearly independent solutions corresponding to this root are x^{λ_1}, $x^{\lambda_1}\ln x, \ldots, x^{\lambda_1}(\ln x)^{k-1}$.

►*Solve*

$$x^2\frac{d^2y}{dx^2}+x\frac{dy}{dx}-4y=0 \qquad (15.39)$$

by both of the methods discussed above.

First we make the substitution $x = e^t$, which, after cancelling e^t, gives an equation with constant coefficients, i.e.

$$\frac{d}{dt}\left(\frac{d}{dt}-1\right)y+\frac{dy}{dt}-4y=0 \quad\Rightarrow\quad \frac{d^2y}{dt^2}-4y=0. \qquad (15.40)$$

Using the methods of section 15.1, the general solution of (15.40), and therefore of (15.39), is given by

$$y=c_1e^{2t}+c_2e^{-2t}=c_1x^2+c_2x^{-2}.$$

Since the RHS of (15.39) is zero, we can reach the same solution by substituting $y = x^\lambda$ into (15.39). This gives

$$\lambda(\lambda-1)x^\lambda+\lambda x^\lambda-4x^\lambda=0,$$

which reduces to

$$(\lambda^2-4)x^\lambda=0.$$

This has the solutions $\lambda = \pm 2$, so we obtain again the general solution

$$y=c_1x^2+c_2x^{-2}. \blacktriangleleft$$

Solution method. *If the ODE is of the Legendre form (15.36) then substitute $\alpha x + \beta = e^t$. This results in an equation of the same order but with constant coefficients, which can be solved by the methods of section 15.1. If the ODE is of the Euler form (15.38) with a non-zero RHS then substitute $x = e^t$; this again leads to an equation of the same order but with constant coefficients. If, however, $f(x) = 0$ in the Euler equation (15.38) then the equation may also be solved by substituting*

$y = x^\lambda$. This leads to an algebraic equation whose solution gives the allowed values of λ; the general solution is then the linear superposition of these functions.

15.2.2 Exact equations

Sometimes an ODE may be merely the derivative of another ODE of one order lower. If this is the case then the ODE is called exact. The nth-order linear ODE

$$a_n(x)\frac{d^n y}{dx^n} + \cdots + a_1(x)\frac{dy}{dx} + a_0(x)y = f(x), \tag{15.41}$$

is exact if the LHS can be written as a simple derivative, i.e. if

$$a_n(x)\frac{d^n y}{dx^n} + \cdots + a_0(x)y = \frac{d}{dx}\left[b_{n-1}(x)\frac{d^{n-1} y}{dx^{n-1}} + \cdots + b_0(x)y\right]. \tag{15.42}$$

It may be shown that, for (15.42) to hold, we require

$$a_0(x) - a_1'(x) + a_2''(x) - \cdots + (-1)^n a_n^{(n)}(x) = 0, \tag{15.43}$$

where the prime again denotes differentiation with respect to x. If (15.43) is satisfied then straightforward integration leads to a new equation of one order lower. If this simpler equation can be solved then a solution to the original equation is obtained. Of course, if the above process leads to an equation that is itself exact then the analysis can be repeated to reduce the order still further.

►*Solve*

$$(1 - x^2)\frac{d^2 y}{dx^2} - 3x\frac{dy}{dx} - y = 1. \tag{15.44}$$

Comparing with (15.41), we have $a_2 = 1 - x^2$, $a_1 = -3x$ and $a_0 = -1$. It is easily shown that $a_0 - a_1' + a_2'' = 0$, so (15.44) is exact and can therefore be written in the form

$$\frac{d}{dx}\left[b_1(x)\frac{dy}{dx} + b_0(x)y\right] = 1. \tag{15.45}$$

Expanding the LHS of (15.45) we find

$$\frac{d}{dx}\left(b_1\frac{dy}{dx} + b_0 y\right) = b_1\frac{d^2 y}{dx^2} + (b_1' + b_0)\frac{dy}{dx} + b_0' y. \tag{15.46}$$

Comparing (15.44) and (15.46) we find

$$b_1 = 1 - x^2, \qquad b_1' + b_0 = -3x, \qquad b_0' = -1.$$

These relations integrate consistently to give $b_1 = 1 - x^2$ and $b_0 = -x$, so (15.44) can be written as

$$\frac{d}{dx}\left[(1 - x^2)\frac{dy}{dx} - xy\right] = 1. \tag{15.47}$$

Integrating (15.47) gives us directly the first-order linear ODE

$$\frac{dy}{dx} - \left(\frac{x}{1 - x^2}\right) y = \frac{x + c_1}{1 - x^2},$$

which can be solved by the method of subsection 14.2.4 and has the solution

$$y = \frac{c_1 \sin^{-1} x + c_2}{\sqrt{1 - x^2}} - 1. \blacktriangleleft$$

It is worth noting that, even if a higher-order ODE is not exact in its given form, it may sometimes be made exact by multiplying through by some suitable function, an *integrating factor*, cf. subsection 14.2.3. Unfortunately, no straightforward method for finding an integrating factor exists and one often has to rely on inspection or experience.

►*Solve*

$$x(1-x^2)\frac{d^2y}{dx^2} - 3x^2\frac{dy}{dx} - xy = x. \tag{15.48}$$

It is easily shown that (15.48) is not exact, but we also see immediately that by multiplying it through by $1/x$ we recover (15.44), which is exact and is solved above. ◄

Another important point is that an ODE need not be linear to be exact, although no simple rule such as (15.43) exists if it is not linear. Nevertheless, it is often worth exploring the possibility that a non-linear equation is exact, since it could then be reduced in order by one and may lead to a soluble equation. This is discussed further in subsection 15.3.3.

Solution method. *For a linear ODE of the form (15.41) check whether it is exact using equation (15.43). If it is not then attempt to find an integrating factor which when multiplying the equation makes it exact. Once the equation is exact write the LHS as a derivative as in (15.42) and, by expanding this derivative and comparing with the LHS of the ODE, determine the functions $b_m(x)$ in (15.42). Integrate the resulting equation to yield another ODE, of one order lower. This may be solved or simplified further if the new ODE is itself exact or can be made so.*

15.2.3 Partially known complementary function

Suppose we wish to solve the nth-order linear ODE

$$a_n(x)\frac{d^ny}{dx^n} + \cdots + a_1(x)\frac{dy}{dx} + a_0(x)y = f(x), \tag{15.49}$$

and we happen to know that $u(x)$ is a solution of (15.49) when the RHS is set to zero, i.e. $u(x)$ is one part of the complementary function. By making the substitution $y(x) = u(x)v(x)$, we can transform (15.49) into an equation of order $n-1$ in dv/dx. This simpler equation may prove soluble.

In particular, if the original equation is of second order then we obtain a first-order equation in dv/dx, which may be soluble using the methods of section 14.2. In this way both the remaining term in the complementary function and the particular integral are found. This method therefore provides a useful way of calculating particular integrals for second-order equations with variable (or constant) coefficients.

►*Solve*

$$\frac{d^2 y}{dx^2} + y = \operatorname{cosec} x. \tag{15.50}$$

We see that the RHS does not fall into any of the categories listed in subsection 15.1.2, and so we are at an initial loss as to how to find the particular integral. However, the complementary function of (15.50) is

$$y_c(x) = c_1 \sin x + c_2 \cos x,$$

and so let us choose the solution $u(x) = \cos x$ (we could equally well choose $\sin x$) and make the substitution $y(x) = v(x)u(x) = v(x)\cos x$ into (15.50). This gives

$$\cos x \frac{d^2 v}{dx^2} - 2 \sin x \frac{dv}{dx} = \operatorname{cosec} x, \tag{15.51}$$

which is a first-order linear ODE in dv/dx and may be solved by multiplying through by a suitable integrating factor, as discussed in subsection 14.2.4. Writing (15.51) as

$$\frac{d^2 v}{dx^2} - 2 \tan x \frac{dv}{dx} = \frac{\operatorname{cosec} x}{\cos x}, \tag{15.52}$$

we see that the required integrating factor is given by

$$\exp\left\{-2 \int \tan x \, dx\right\} = \exp\left[2 \ln(\cos x)\right] = \cos^2 x.$$

Multiplying both sides of (15.52) by the integrating factor $\cos^2 x$ we obtain

$$\frac{d}{dx}\left(\cos^2 x \frac{dv}{dx}\right) = \cot x,$$

which integrates to give

$$\cos^2 x \frac{dv}{dx} = \ln(\sin x) + c_1.$$

After rearranging and integrating again, this becomes

$$\begin{aligned} v &= \int \sec^2 x \ln(\sin x)\, dx + c_1 \int \sec^2 x \, dx \\ &= \tan x \ln(\sin x) - x + c_1 \tan x + c_2. \end{aligned}$$

Therefore the general solution to (15.50) is given by $y = uv = v \cos x$, i.e.

$$y = c_1 \sin x + c_2 \cos x + \sin x \ln(\sin x) - x \cos x,$$

which contains the full complementary function and the particular integral. ◄

Solution method. *If $u(x)$ is a known solution of the nth-order equation (15.49) with $f(x) = 0$, then make the substitution $y(x) = u(x)v(x)$ in (15.49). This leads to an equation of order $n - 1$ in dv/dx, which might be soluble.*

15.2.4 Variation of parameters

The method of variation of parameters proves useful in finding particular integrals for linear ODEs with variable (and constant) coefficients. However, it requires knowledge of the entire complementary function, not just of one part of it as in the previous subsection.

Suppose we wish to find a particular integral of the equation

$$a_n(x)\frac{d^n y}{dx^n} + \cdots + a_1(x)\frac{dy}{dx} + a_0(x)y = f(x), \tag{15.53}$$

and the complementary function $y_c(x)$ (the general solution of (15.53) with $f(x) = 0$) is

$$y_c(x) = c_1 y_1(x) + c_2 y_2(x) + \cdots + c_n y_n(x),$$

where the functions $y_m(x)$ are known. We now assume that a particular integral of (15.53) can be expressed in a form similar to that of the complementary function, but with the constants c_m replaced by functions of x, i.e. we assume a particular integral of the form

$$y_p(x) = k_1(x)y_1(x) + k_2(x)y_2(x) + \cdots + k_n(x)y_n(x). \tag{15.54}$$

This will no longer satisfy the complementary equation (i.e. (15.53) with the RHS set to zero) but might, with suitable choices of the functions $k_i(x)$, be made equal to $f(x)$, thus producing not a complementary function but a particular integral.

Since we have n arbitrary functions $k_1(x), k_2(x), \ldots, k_n(x)$, but only one restriction on them (namely the ODE), we may impose a further $n-1$ constraints. We can choose these constraints to be as convenient as possible, and the simplest choice is given by

$$\begin{aligned}
k_1'(x)y_1(x) + k_2'(x)y_2(x) + \cdots + k_n'(x)y_n(x) &= 0 \\
k_1'(x)y_1'(x) + k_2'(x)y_2'(x) + \cdots + k_n'(x)y_n'(x) &= 0 \\
&\;\vdots \\
k_1'(x)y_1^{(n-2)}(x) + k_2'(x)y_2^{(n-2)}(x) + \cdots + k_n'(x)y_n^{(n-2)}(x) &= 0 \\
k_1'(x)y_1^{(n-1)}(x) + k_2'(x)y_2^{(n-1)}(x) + \cdots + k_n'(x)y_n^{(n-1)}(x) &= \frac{f(x)}{a_n(x)},
\end{aligned} \tag{15.55}$$

where the primes denote differentiation with respect to x. The last of these equations is not a freely chosen constraint; given the previous $n-1$ constraints and the original ODE, it must be satisfied.

This choice of constraints is easily justified (although the algebra is quite messy). Differentiating (15.54) with respect to x, we obtain

$$y_p' = k_1 y_1' + k_2 y_2' + \cdots + k_n y_n' + [\,k_1' y_1 + k_2' y_2 + \cdots + k_n' y_n\,],$$

where, for the moment, we drop the explicit x-dependence of these functions. Since we are free to choose our constraints as we wish, let us define the expression in parentheses to be zero, giving the first equation in (15.55). Differentiating again we find

$$y_{\rm p}'' = k_1 y_1'' + k_2 y_2'' + \cdots + k_n y_n'' + [k_1' y_1' + k_2' y_2' + \cdots + k_n' y_n'].$$

Once more we can choose the expression in brackets to be zero, giving the second equation in (15.55). We can repeat this procedure, choosing the corresponding expression in each case to be zero. This yields the first $n-1$ equations in (15.55). The mth derivative of $y_{\rm p}$ for $m < n$ is then given by

$$y_{\rm p}^{(m)} = k_1 y_1^{(m)} + k_2 y_2^{(m)} + \cdots + k_n y_n^{(m)}.$$

Differentiating $y_{\rm p}$ once more we find that its nth derivative is given by

$$y_{\rm p}^{(n)} = k_1 y_1^{(n)} + k_2 y_2^{(n)} + \cdots + k_n y_n^{(n)} + [k_1' y_1^{(n-1)} + k_2' y_2^{(n-1)} + \cdots + k_n' y_n^{(n-1)}].$$

Substituting the expressions for $y_{\rm p}^{(m)}$, $m = 0$ to n, into the original ODE (15.53), we obtain

$$\sum_{m=0}^{n} a_m [k_1 y_1^{(m)} + k_2 y_2^{(m)} + \cdots + k_n y_n^{(m)}] + a_n [k_1' y_1^{(n-1)} + k_2' y_2^{(n-1)} + \cdots + k_n' y_n^{(n-1)}] = f(x),$$

i.e.

$$\sum_{m=0}^{n} a_m \sum_{j=1}^{n} k_j y_j^{(m)} + a_n [k_1' y_1^{(n-1)} + k_2' y_2^{(n-1)} + \cdots + k_n' y_n^{(n-1)}] = f(x).$$

Rearranging the order of summation on the LHS, we find

$$\sum_{j=1}^{n} k_j [a_n y_j^{(n)} + \cdots + a_1 y_j' + a_0 y_j] + a_n [k_1' y_1^{(n-1)} + k_2' y_2^{(n-1)} + \cdots + k_n' y_n^{(n-1)}] = f(x). \qquad (15.56)$$

But since the functions y_j are solutions of the complementary equation of (15.53) we have (for all j)

$$a_n y_j^{(n)} + \cdots + a_1 y_j' + a_0 y_j = 0.$$

Therefore (15.56) becomes

$$a_n [k_1' y_1^{(n-1)} + k_2' y_2^{(n-1)} + \cdots + k_n' y_n^{(n-1)}] = f(x),$$

which is the final equation given in (15.55).

Considering (15.55) to be a set of simultaneous equations in the set of unknowns $k_1'(x), k_2', \ldots, k_n'(x)$, we see that the determinant of the coefficients of these functions is equal to the Wronskian $W(y_1, y_2, \ldots, y_n)$, which is non-zero since the solutions $y_m(x)$ are linearly independent; see equation (15.6). Therefore (15.55) can be solved for the functions $k_m'(x)$, which in turn can be integrated, setting all constants of integration equal to zero, to give $k_m(x)$. The general solution to (15.53) is then given by

$$y(x) = y_c(x) + y_p(x) = \sum_{m=1}^{n} [c_m + k_m(x)]\, y_m(x).$$

Note that if the constants of integration are included in the $k_m(x)$ then, as well as finding the particular integral, we redefine the arbitrary constants c_m in the complementary function.

►*Use the variation-of-parameters method to solve*

$$\frac{d^2 y}{dx^2} + y = \operatorname{cosec} x, \tag{15.57}$$

subject to the boundary conditions $y(0) = y(\pi/2) = 0$.

The complementary function of (15.57) is again

$$y_c(x) = c_1 \sin x + c_2 \cos x.$$

We therefore assume a particular integral of the form

$$y_p(x) = k_1(x) \sin x + k_2(x) \cos x,$$

and impose the additional constraints of (15.55), i.e.

$$k_1'(x) \sin x + k_2'(x) \cos x = 0,$$
$$k_1'(x) \cos x - k_2'(x) \sin x = \operatorname{cosec} x.$$

Solving these equations for $k_1'(x)$ and $k_2'(x)$ gives

$$k_1'(x) = \cos x \operatorname{cosec} x = \cot x,$$
$$k_2'(x) = -\sin x \operatorname{cosec} x = -1.$$

Hence, ignoring the constants of integration, $k_1(x)$ and $k_2(x)$ are given by

$$k_1(x) = \ln(\sin x),$$
$$k_2(x) = -x.$$

The general solution to the ODE (15.57) is therefore

$$y(x) = [c_1 + \ln(\sin x)] \sin x + (c_2 - x) \cos x,$$

which is identical to the solution found in subsection 15.2.3. Applying the boundary conditions $y(0) = y(\pi/2) = 0$ we find $c_1 = c_2 = 0$ and so

$$y(x) = \ln(\sin x) \sin x - x \cos x. \blacktriangleleft$$

Solution method. *If the complementary function of (15.53) is known then assume a particular integral of the same form but with the constants replaced by functions of x. Impose the constraints in (15.55) and solve the resulting system of equations for the unknowns* $k_1'(x), k_2', \ldots, k_n'(x)$. *Integrate these functions, setting constants of integration equal to zero, to obtain* $k_1(x), k_2(x), \ldots, k_n(x)$ *and hence the particular integral.*

15.2.5 Green's functions

The Green's function method of solving linear ODEs bears a striking resemblance to the method of variation of parameters discussed in the previous subsection; it too requires knowledge of the entire complementary function in order to find the particular integral and therefore the general solution. The Green's function approach differs, however, since once the Green's function for a particular LHS of (15.1) and particular boundary conditions has been found, then the solution for *any* RHS (i.e. any $f(x)$) can be written down immediately, albeit in the form of an integral.

Although the Green's function method can be approached by considering the superposition of eigenfunctions of the equation (see chapter 17) and is also applicable to the solution of partial differential equations (see chapter 21), this section adopts a more utilitarian approach based on the properties of the Dirac delta function (see subsection 13.1.3) and deals only with the use of Green's functions in solving ODEs.

Let us again consider the equation

$$a_n(x)\frac{d^n y}{dx^n} + \cdots + a_1(x)\frac{dy}{dx} + a_0(x)y = f(x), \qquad (15.58)$$

but for the sake of brevity we now denote the LHS by $\mathcal{L}y(x)$, i.e. as a linear differential operator acting on $y(x)$. Thus (15.58) now reads

$$\mathcal{L}y(x) = f(x). \qquad (15.59)$$

Let us suppose that a function $G(x,z)$ (the *Green's function*) exists such that the general solution to (15.59), which obeys some set of imposed boundary conditions in the range $a \le x \le b$, is given by

$$y(x) = \int_a^b G(x,z)f(z)\,dz, \qquad (15.60)$$

where z is the integration variable. If we apply the linear differential operator $\mathcal{L}$ to both sides of (15.60) and use (15.59) then we obtain

$$\mathcal{L}y(x) = \int_a^b [\mathcal{L}G(x,z)]\,f(z)\,dz = f(x). \qquad (15.61)$$

Comparison of (15.61) with a standard property of the Dirac delta function (see subsection 13.1.3), namely

$$f(x) = \int_a^b \delta(x-z)f(z)\,dz,$$

for $a \le x \le b$, shows that for (15.61) to hold for any arbitrary function $f(x)$, we require (for $a \le x \le b$) that

$$\mathcal{L}G(x,z) = \delta(x-z), \qquad (15.62)$$

i.e. the Green's function $G(x,z)$ must satisfy the original ODE with the RHS set equal to a delta function. $G(x,z)$ may be thought of physically as the response of a system to a unit impulse at $x=z$.

In addition to (15.62), we must impose two further sets of restrictions on $G(x,z)$. The first is the requirement that the general solution $y(x)$ in (15.60) obeys the boundary conditions. For *homogeneous* boundary conditions, in which $y(x)$ and/or its derivatives are required to be *zero* at specified points, this is most simply arranged by demanding that $G(x,z)$ itself obeys the boundary conditions when it is considered as a function of x alone; if, for example, we require $y(a) = y(b) = 0$ then we should also demand $G(a,z) = G(b,z) = 0$. Problems having inhomogeneous boundary conditions are discussed at the end of this subsection.

The second set of restrictions concerns the continuity or discontinuity of $G(x,z)$ and its derivatives at $x=z$ and can be found by integrating (15.62) with respect to x over the small interval $[z-\epsilon,\ z+\epsilon]$ and taking the limit as $\epsilon \to 0$. We then obtain

$$\lim_{\epsilon\to 0}\sum_{m=0}^{n}\int_{z-\epsilon}^{z+\epsilon} a_m(x)\frac{d^mG(x,z)}{dx^m}\,dx = \lim_{\epsilon\to 0}\int_{z-\epsilon}^{z+\epsilon}\delta(x-z)\,dx = 1. \tag{15.63}$$

Since d^nG/dx^n exists at $x=z$ but with value infinity, the $(n-1)$th-order derivative must have a finite discontinuity there, whereas all the lower-order derivatives, d^mG/dx^m for $m < n-1$, must be continuous at this point. Therefore the terms containing these derivatives cannot contribute to the value of the integral on the LHS of (15.63). Noting that, apart from an arbitrary additive constant, $\int (d^mG/dx^m)\,dx = d^{m-1}G/dx^{m-1}$, and integrating the terms on the LHS of (15.63) by parts we find

$$\lim_{\epsilon\to 0}\int_{z-\epsilon}^{z+\epsilon} a_m(x)\frac{d^mG(x,z)}{dx^m}\,dx = 0 \tag{15.64}$$

for $m=0$ to $n-1$. Thus, since only the term containing d^nG/dx^n contributes to the integral in (15.63), we conclude, after performing an integration by parts, that

$$\lim_{\epsilon\to 0}\left[a_n(x)\frac{d^{n-1}G(x,z)}{dx^{n-1}}\right]_{z-\epsilon}^{z+\epsilon} = 1. \tag{15.65}$$

Thus we have the further n constraints that $G(x,z)$ and its derivatives up to order $n-2$ are continuous at $x=z$ but that $d^{n-1}G/dx^{n-1}$ has a discontinuity of $1/a_n(z)$ at $x=z$.

Thus the properties of the Green's function $G(x,z)$ for an nth-order linear ODE may be summarised by the following.

(i) $G(x,z)$ obeys the original ODE but with $f(x)$ on the RHS set equal to a delta function $\delta(x-z)$.

(ii) When considered as a function of x alone $G(x,z)$ obeys the specified (homogeneous) boundary conditions on $y(x)$.

(iii) The derivatives of $G(x,z)$ with respect to x up to order $n-2$ are continuous at $x=z$, but the $(n-1)$th-order derivative has a discontinuity of $1/a_n(z)$ at this point.

►*Use Green's functions to solve*

$$\frac{d^2y}{dx^2}+y=\operatorname{cosec} x, \tag{15.66}$$

subject to the boundary conditions $y(0)=y(\pi/2)=0$.

From (15.62) we see that the Green's function $G(x,z)$ must satisfy

$$\frac{d^2G(x,z)}{dx^2}+G(x,z)=\delta(x-z). \tag{15.67}$$

Now it is clear that for $x\neq z$ the RHS of (15.67) is zero, and we are left with the task of finding the general solution to the homogeneous equation, i.e. the complementary function. The complementary function of (15.67) consists of a linear superposition of $\sin x$ and $\cos x$ and *must* consist of different superpositions on either side of $x=z$, since its $(n-1)$th derivative (i.e. the first derivative in this case) is required to have a discontinuity there. Therefore we assume the form of the Green's function to be

$$G(x,z)=\begin{cases}A(z)\sin x+B(z)\cos x & \text{for } x<z,\\ C(z)\sin x+D(z)\cos x & \text{for } x>z.\end{cases}$$

Note that we have performed a similar (but not identical) operation to that used in the variation-of-parameters method, i.e. we have replaced the constants in the complementary function with functions (this time of z).

We must now impose the relevant restrictions on $G(x,z)$ in order to determine the functions $A(z),\ldots,D(z)$. The first of these is that $G(x,z)$ should itself obey the homogeneous boundary conditions $G(0,z)=G(\pi/2,z)=0$. This leads to the conclusion that $B(z)=C(z)=0$, so we now have

$$G(x,z)=\begin{cases}A(z)\sin x & \text{for } x<z,\\ D(z)\cos x & \text{for } x>z.\end{cases}$$

The second restriction is the continuity conditions given in equations (15.64), (15.65), namely that, for this second-order equation, $G(x,z)$ is continuous at $x=z$ and dG/dx has a discontinuity of $1/a_2(z)=1$ at this point. Applying these two constraints we have

$$\begin{aligned}D(z)\cos z-A(z)\sin z&=0\\ -D(z)\sin z-A(z)\cos z&=1.\end{aligned}$$

Solving these equations for $A(z)$ and $D(z)$, we find

$$A(z)=-\cos z,\qquad D(z)=-\sin z.$$

Thus we have

$$G(x,z)=\begin{cases}-\cos z\sin x & \text{for } x<z,\\ -\sin z\cos x & \text{for } x>z.\end{cases}$$

Therefore, from (15.60), the general solution to (15.66) that obeys the boundary conditions

$y(0) = y(\pi/2) = 0$ is given by

$$\begin{aligned} y(x) &= \int_0^{\pi/2} G(x,z)\,\mathrm{cosec}\, z\, dz \\ &= -\cos x \int_0^x \sin z\,\mathrm{cosec}\, z\, dz - \sin x \int_x^{\pi/2} \cos z\,\mathrm{cosec}\, z\, dz \\ &= -x\cos x + \sin x \ln(\sin x), \end{aligned}$$

which agrees with the result obtained in the previous subsections. ◀

As mentioned earlier, once a Green's function has been obtained for a given LHS and boundary conditions, it can be used to find a general solution for any RHS; thus, the solution of $d^2y/dx^2 + y = f(x)$, with $y(0) = y(\pi/2) = 0$, is given immediately by

$$\begin{aligned} y(x) &= \int_0^{\pi/2} G(x,z) f(z)\, dz \\ &= -\cos x \int_0^x \sin z\; f(z)\, dz - \sin x \int_x^{\pi/2} \cos z\; f(z)\, dz. \end{aligned} \tag{15.68}$$

As an example, the reader may wish to verify that if $f(x) = \sin 2x$ then (15.68) gives $y(x) = (-\sin 2x)/3$, a solution easily verified by direct substitution. In general, analytic integration of (15.68) for arbitrary $f(x)$ will prove intractable; then the integrals must be evaluated numerically.

Another important point is that although the Green's function method above has provided a general solution, it is also useful for finding a particular integral if the complementary function is known. This is easily seen since in (15.68) the constant integration limits 0 and $\pi/2$ lead merely to constant values by which the factors $\sin x$ and $\cos x$ are multiplied; thus the complementary function is reconstructed. The rest of the general solution, i.e. the particular integral, comes from the variable integration limit x. Therefore by changing $\int_x^{\pi/2}$ to $-\int^x$, and so dropping the constant integration limits, we can find just the particular integral. For example, a particular integral of $d^2y/dx^2 + y = f(x)$ that satisfies the above boundary conditions is given by

$$y_{\mathrm{p}}(x) = -\cos x \int^x \sin z\; f(z)\, dz + \sin x \int^x \cos z\; f(z)\, dz.$$

A very important point to realise about the Green's function method is that a particular $G(x,z)$ applies to a given LHS of an ODE *and* the imposed boundary conditions, i.e. *the same equation with different boundary conditions will have a different Green's function.* To illustrate this point, let us consider again the ODE solved in (15.68), but with different boundary conditions.

►*Use Green's functions to solve*

$$\frac{d^2y}{dx^2} + y = f(x), \tag{15.69}$$

subject to the one-point boundary conditions $y(0) = y'(0) = 0$.

We again require (15.67) to hold and so again we assume a Green's function of the form

$$G(x,z) = \begin{cases} A(z)\sin x + B(z)\cos x & \text{for } x < z, \\ C(z)\sin x + D(z)\cos x & \text{for } x > z. \end{cases}$$

However, we now require $G(x,z)$ to obey the boundary conditions $G(0,z) = G'(0,z) = 0$, which imply $A(z) = B(z) = 0$. Therefore we have

$$G(x,z) = \begin{cases} 0 & \text{for } x < z, \\ C(z)\sin x + D(z)\cos x & \text{for } x > z. \end{cases}$$

Applying the continuity conditions on $G(x,z)$ as before now gives

$$C(z)\sin z + D(z)\cos z = 0,$$
$$C(z)\cos z - D(z)\sin z = 1,$$

which are solved to give

$$C(z) = \cos z, \qquad D(z) = -\sin z.$$

So finally the Green's function is given by

$$G(x,z) = \begin{cases} 0 & \text{for } x < z, \\ \sin(x-z) & \text{for } x > z, \end{cases}$$

and the general solution to (15.69) that obeys the boundary conditions $y(0) = y'(0) = 0$ is

$$\begin{aligned} y(x) &= \int_0^\infty G(x,z)f(z)\,dz \\ &= \int_0^x \sin(x-z)f(z)\,dz. \end{aligned}$$ ◄

Finally, we consider how to deal with inhomogeneous boundary conditions such as $y(a) = \alpha$, $y(b) = \beta$ or $y(0) = y'(0) = \gamma$, where α, β, γ are non-zero. The simplest method of solution in this case is to make a change of variable such that the boundary conditions in the new variable, u say, are homogeneous, i.e. $u(a) = u(b) = 0$ or $u(0) = u'(0) = 0$ etc. For nth-order equations we generally require n boundary conditions to fix the solution, but these n boundary conditions can be of various types: we could have the n-point boundary conditions $y(x_m) = y_m$ for $m = 1$ to n, or the one-point boundary conditions $y(x_0) = y'(x_0) = \cdots = y^{(n-1)}(x_0) = y_0$, or something in between. In all cases a suitable change of variable is

$$u = y - h(x),$$

where $h(x)$ is an $(n-1)$th-order polynomial that obeys the boundary conditions.

For example, if we consider the second-order case with boundary conditions $y(a) = \alpha$, $y(b) = \beta$ then a suitable change of variable is

$$u = y - (mx + c),$$

where $y = mx + c$ is the straight line through the points (a, α) and (b, β), for which $m = (\alpha - \beta)/(a - b)$ and $c = (\beta a - \alpha b)/(a - b)$. Alternatively, if the boundary conditions for our second-order equation are $y(0) = y'(0) = \gamma$ then we would make the same change of variable, but this time $y = mx + c$ would be the straight line through $(0, \gamma)$ with slope γ, i.e. $m = c = \gamma$.

Solution method. *Require that the Green's function $G(x, z)$ obeys the original ODE, but with the RHS set to a delta function $\delta(x - z)$. This is equivalent to assuming that $G(x, z)$ is given by the complementary function of the original ODE, with the constants replaced by functions of z; these functions are different for $x < z$ and $x > z$. Now require also that $G(x, z)$ obeys the given homogeneous boundary conditions and impose the continuity conditions given in (15.64) and (15.65). The general solution to the original ODE is then given by (15.60). For inhomogeneous boundary conditions, make the change of dependent variable $u = y - h(x)$, where $h(x)$ is a polynomial obeying the given boundary conditions.*

15.2.6 Canonical form for second-order equations

In this section we specialise from nth-order linear ODEs with variable coefficients to those of order 2. In particular we consider the equation

$$\frac{d^2y}{dx^2} + a_1(x)\frac{dy}{dx} + a_0(x)y = f(x), \tag{15.70}$$

which has been rearranged so that the coefficient of d^2y/dx^2 is unity. By making the substitution $y(x) = u(x)v(x)$ we obtain

$$v'' + \left(\frac{2u'}{u} + a_1\right)v' + \left(\frac{u'' + a_1u' + a_0u}{u}\right)v = \frac{f}{u}, \tag{15.71}$$

where the prime denotes differentiation with respect to x. Since (15.71) would be much simplified if there were no term in v', let us choose $u(x)$ such that the first factor in parentheses on the LHS of (15.71) is zero, i.e.

$$\frac{2u'}{u} + a_1 = 0 \qquad \Rightarrow \qquad u(x) = \exp\left\{-\tfrac{1}{2}\int a_1(z)\,dz\right\}. \tag{15.72}$$

We then obtain an equation of the form

$$\frac{d^2v}{dx^2} + g(x)v = h(x), \tag{15.73}$$

where

$$g(x) = a_0(x) - \tfrac{1}{4}[a_1(x)]^2 - \tfrac{1}{2}a_1'(x)$$
$$h(x) = f(x)\exp\left\{\tfrac{1}{2}\int a_1(z)\,dz\right\}.$$

Since (15.73) is of a simpler form than the original equation, (15.70), it may prove easier to solve.

►*Solve*

$$4x^2\frac{d^2y}{dx^2} + 4x\frac{dy}{dx} + (x^2 - 1)y = 0. \qquad (15.74)$$

Dividing (15.74) through by $4x^2$, we see that it is of the form (15.70) with $a_1(x) = 1/x$, $a_0(x) = (x^2 - 1)/4x^2$ and $f(x) = 0$. Therefore, making the substitution

$$y = vu = v\exp\left(-\int \frac{1}{2x}\,dx\right) = \frac{Av}{\sqrt{x}},$$

we obtain

$$\frac{d^2v}{dx^2} + \frac{v}{4} = 0. \qquad (15.75)$$

Equation (15.75) is easily solved to give

$$v = c_1 \sin \tfrac{1}{2}x + c_2 \cos \tfrac{1}{2}x,$$

so the solution of (15.74) is

$$y = \frac{v}{\sqrt{x}} = \frac{c_1 \sin \frac{1}{2}x + c_2 \cos \frac{1}{2}x}{\sqrt{x}}. \blacktriangleleft$$

As an alternative to choosing $u(x)$ such that the coefficient of v' in (15.71) is zero, we could choose a different $u(x)$ such that the coefficient of v vanishes. For this to be the case, we see from (15.71) that we would require

$$u'' + a_1u' + a_0u = 0,$$

so $u(x)$ would have to be a solution of the original ODE with the RHS set to zero, i.e. part of the complementary function. If such a solution were known then the substitution $y = uv$ would yield an equation with no term in v, which could be solved by two straightforward integrations. This is a special (second-order) case of the method discussed in subsection 15.2.3.

Solution method. *Write the equation in the form (15.70), then substitute $y = uv$, where $u(x)$ is given by (15.72). This leads to an equation of the form (15.73), in which there is no term in dv/dx and which may be easier to solve. Alternatively, if part of the complementary function is known then follow the method of subsection 15.2.3.*

15.3 General ordinary differential equations

In this section, we discuss miscellaneous methods for simplifying general ODEs. These methods are applicable to both linear and non-linear equations and in some cases may lead to a solution. More often than not, however, finding a closed-form solution to a general non-linear ODE proves impossible.

15.3.1 Dependent variable absent

If an ODE does not contain the dependent variable y explicitly, but only its derivatives, then the change of variable $p = dy/dx$ leads to an equation of one order lower.

►*Solve*

$$\frac{d^2y}{dx^2} + 2\frac{dy}{dx} = 4x \tag{15.76}$$

This is transformed by the substitution $p = dy/dx$ to the first-order equation

$$\frac{dp}{dx} + 2p = 4x. \tag{15.77}$$

The solution to (15.77) is then found by the method of subsection 14.2.4 and reads

$$p = \frac{dy}{dx} = ae^{-2x} + 2x - 1,$$

where a is a constant. Thus by direct integration the solution to the original equation, (15.76), is

$$y(x) = c_1e^{-2x} + x^2 - x + c_2. \blacktriangleleft$$

An extension to the above method is appropriate if an ODE contains only derivatives of y that are of order m and greater. Then the substitution $p = d^my/dx^m$ reduces the order of the ODE by m.

Solution method. *If the ODE contains only derivatives of y that are of order m and greater then the substitution $p = d^my/dx^m$ reduces the order of the equation by m.*

15.3.2 Independent variable absent

If an ODE does not contain the independent variable x explicitly, except in d/dx, d^2/dx^2 etc., then as in the previous subsection we make the substitution $p = dy/dx$

but also write

$$\frac{d^2y}{dx^2} = \frac{dp}{dx} = \frac{dy}{dx}\frac{dp}{dy} = p\frac{dp}{dy}$$
$$\frac{d^3y}{dx^3} = \frac{d}{dx}\left(p\frac{dp}{dy}\right) = \frac{dy}{dx}\frac{d}{dy}\left(p\frac{dp}{dy}\right) = p^2\frac{d^2p}{dy^2} + p\left(\frac{dp}{dy}\right)^2, \qquad (15.78)$$

and so on for higher-order derivatives. This leads to an equation of one order lower.

►*Solve*

$$1 + y\frac{d^2y}{dx^2} + \left(\frac{dy}{dx}\right)^2 = 0. \qquad (15.79)$$

Making the substitutions $dy/dx = p$ and $d^2y/dx^2 = p(dp/dy)$ we obtain the first-order ODE

$$1 + yp\frac{dp}{dy} + p^2 = 0,$$

which is separable and may be solved as in subsection 14.2.1 to obtain

$$(1 + p^2)y^2 = c_1.$$

Using $p = dy/dx$ we therefore have

$$p = \frac{dy}{dx} = \pm\sqrt{\frac{c_1^2 - y^2}{y^2}},$$

which may be integrated to give the general solution of (15.79); after squaring this reads

$$(x + c_2)^2 + y^2 = c_1^2. \blacktriangleleft$$

Solution method. *If the ODE does not contain x explicitly then substitute $p = dy/dx$, along with the relations for higher derivatives given in (15.78), to obtain an equation of one order lower, which may prove easier to solve.*

15.3.3 Non-linear exact equations

As discussed in subsection 15.2.2, an exact ODE is one that can be obtained by straightforward differentiation of an equation of one order lower. Moreover, the notion of exact equations is useful for both linear and non-linear equations, since an exact equation can be immediately integrated. It is possible, of course, that the resulting equation may itself be exact, so that the process can be repeated. In the non-linear case, however, there is no simple relation (such as (15.43) for the linear case) by which an equation can be shown to be exact. Nevertheless, a general procedure does exist and is illustrated in the following example.

►*Solve*

$$2y\frac{d^3y}{dx^3} + 6\frac{dy}{dx}\frac{d^2y}{dx^2} = x. \tag{15.80}$$

Directing our attention to the term on the LHS of (15.80) that contains the highest-order derivative, i.e. $2y\, d^3y/dx^3$, we see that it can be obtained by differentiating $2y\, d^2y/dx^2$ since

$$\frac{d}{dx}\left(2y\frac{d^2y}{dx^2}\right) = 2y\frac{d^3y}{dx^3} + 2\frac{dy}{dx}\frac{d^2y}{dx^2}. \tag{15.81}$$

Rewriting the LHS of (15.80) using (15.81), we are left with $4(dy/dx)(d^2y/dy^2)$, which may itself be written as a derivative, i.e.

$$4\frac{dy}{dx}\frac{d^2y}{dx^2} = \frac{d}{dx}\left[2\left(\frac{dy}{dx}\right)^2\right]. \tag{15.82}$$

Since, therefore, we can write the LHS of (15.80) as a sum of simple derivatives of other functions, (15.80) is exact. Integrating (15.80) with respect to x, and using (15.81) and (15.82), now gives

$$2y\frac{d^2y}{dx^2} + 2\left(\frac{dy}{dx}\right)^2 = \int x\, dx = \frac{x^2}{2} + c_1. \tag{15.83}$$

Now we can repeat the process to find whether (15.83) is itself exact. Considering the term on the LHS of (15.83) that contains the highest-order derivative, i.e. $2y\, d^2y/dx^2$, we note that we obtain this by differentiating $2y\, dy/dx$, as follows:

$$\frac{d}{dx}\left(2y\frac{dy}{dx}\right) = 2y\frac{d^2y}{dx^2} + 2\left(\frac{dy}{dx}\right)^2.$$

The above expression already contains all the terms on the LHS of (15.83), so we can integrate (15.83) to give

$$2y\frac{dy}{dx} = \frac{x^3}{6} + c_1x + c_2.$$

Integrating once more we obtain the solution

$$y^2 = \frac{x^4}{24} + \frac{c_1x^2}{2} + c_2x + c_3. \blacktriangleleft$$

It is worth noting that both linear equations (as discussed in subsection 15.2.2) and non-linear equations may sometimes be made exact by multiplying through by an appropriate integrating factor. Although no general method exists for finding such a factor, one may sometimes be found by inspection or inspired guesswork.

Solution method. *Rearrange the equation so that all the terms containing y or its derivatives are on the LHS, then check to see whether the equation is exact by attempting to write the LHS as a simple derivative. If this is possible then the equation is exact and may be integrated directly to give an equation of one order lower. If the new equation is itself exact the process can be repeated.*

15.3.4 Isobaric or homogeneous equations

It is straightforward to generalise the discussion of first-order isobaric equations given in subsection 14.2.6 to equations of general order n. An nth-order isobaric equation is one in which every term can be made dimensionally consistent upon giving y and dy each a weight m, and x and dx each a weight 1. Then the nth derivative of y with respect to x, for example, would have dimensions m in y and $-n$ in x. In the special case $m = 1$, for which the equation is dimensionally consistent, the equation is called homogeneous (not to be confused with linear equations with a zero RHS). If an equation is isobaric or homogeneous then the change in dependent variable $y = vx^m$ ($y = vx$ in the homogeneous case) followed by the change in independent variable $x = e^t$ leads to an equation in which the new independent variable t is absent except in the form d/dt.

►*Solve*

$$x^3\frac{d^2y}{dx^2} - (x^2 + xy)\frac{dy}{dx} + (y^2 + xy) = 0. \tag{15.84}$$

Assigning y and dy the weight m, and x and dx the weight 1, the weights of the five terms on the LHS of (15.84) are, from left to right: $m + 1$, $m + 1$, $2m$, $2m$, $m + 1$. For these weights all to be equal we require $m = 1$; thus (15.84) is a homogeneous equation. Since it is homogeneous we now make the substitution $y = vx$, which, after dividing the resulting equation through by x^3, gives

$$x\frac{d^2v}{dx^2} + (1 - v)\frac{dv}{dx} = 0. \tag{15.85}$$

Now substituting $x = e^t$ into (15.85) we obtain (after some working)

$$\frac{d^2v}{dt^2} - v\frac{dv}{dt} = 0, \tag{15.86}$$

which can be integrated directly to give

$$\frac{dv}{dt} = \tfrac{1}{2}v^2 + c_1. \tag{15.87}$$

Equation (15.87) is separable, and integrates to give

$$\begin{aligned}\tfrac{1}{2}t + d_2 &= \int \frac{dv}{v^2 + d_1^2} \\ &= \frac{1}{d_1}\tan^{-1}\left(\frac{v}{d_1}\right).\end{aligned}$$

Rearranging and using $x = e^t$ and $y = vx$ we finally obtain the solution to (15.84) as

$$y = d_1 x \tan\left(\tfrac{1}{2}d_1 \ln x + d_1 d_2\right). \text{ ◄}$$

Solution method. *Assume that y and dy have weight m, and x and dx weight 1, and write down the combined weights of each term in the ODE. If these weights can be made equal by assuming a particular value for m then the equation is isobaric (or homogeneous if $m = 1$). Making the substitution $y = vx^m$ followed by $x = e^t$ leads to an equation in which the new independent variable t is absent except in the form d/dt.*

15.3.5 Equations homogeneous in x or y alone

It will be seen that the intermediate equation (15.85) in the example of the previous subsection was simplified by the substitution $x = e^t$, in that this led to an equation in which the new independent variable t occurred only in the form d/dt; see (15.86). A closer examination of (15.85) reveals that it is dimensionally consistent in the independent variable x *taken alone*; this is equivalent to giving the dependent variable and its differential a weight $m = 0$. For any equation that is homogeneous in x alone, the substitution $x = e^t$ will lead to an equation that does not contain the new independent variable t except as d/dt. Note that the Euler equation of subsection 15.2.1 is a special, linear example of an equation homogeneous in x alone. Similarly, if an equation is homogeneous in y alone, then substituting $y = e^v$ leads to an equation in which the new dependent variable, v, occurs only in the form d/dv.

►*Solve*

$$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} + \frac{2}{y^3} = 0.$$

This equation is homogeneous in x alone, and on substituting $x = e^t$ we obtain

$$\frac{d^2y}{dt^2} + \frac{2}{y^3} = 0,$$

which does not contain the new independent variable t except as d/dt. Such equations may often be solved by the method of subsection 15.3.2, but in this case we can integrate directly to obtain

$$\frac{dy}{dt} = \sqrt{2(c_1 + 1/y^2)}.$$

This equation is separable, and we find

$$\int \frac{dy}{\sqrt{2(c_1 + 1/y^2)}} = t + c_2.$$

By multiplying the numerator and denominator of the integrand on the LHS by y, we find the solution

$$\frac{\sqrt{c_1 y^2 + 1}}{\sqrt{2}c_1} = t + c_2.$$

Remembering that $t = \ln x$, we finally obtain

$$\frac{\sqrt{c_1 y^2 + 1}}{\sqrt{2}c_1} = \ln x + c_2. \blacktriangleleft$$

Solution method. *If the weight of x taken alone is the same in every term in the ODE then the substitution $x = e^t$ leads to an equation in which the new independent variable t is absent except in the form d/dt. If the weight of y taken alone is the same in every term then the substitution $y = e^v$ leads to an equation in which the new dependent variable v is absent except in the form d/dv.*

15.3.6 *Equations having $y = Ae^x$ as a solution*

Finally, we note that if any general (linear or non-linear) nth-order ODE is satisfied identically by assuming that

$$y = \frac{dy}{dx} = \cdots = \frac{d^n y}{dx^n} \tag{15.88}$$

then $y = Ae^x$ is a solution of that equation. This must be so because $y = Ae^x$ is a non-zero function that satisfies (15.88).

►*Find a solution of*

$$(x^2 + x)\frac{dy}{dx}\frac{d^2y}{dx^2} - x^2 y\frac{dy}{dx} - x\left(\frac{dy}{dx}\right)^2 = 0. \tag{15.89}$$

Setting $y = dy/dx = d^2y/dx^2$ in (15.89), we obtain

$$(x^2 + x)y^2 - x^2y^2 - xy^2 = 0,$$

which is satisfied identically. Therefore $y = Ae^x$ is a solution of (15.89); this is easily verified by directly substituting $y = Ae^x$ into (15.89). ◄

Solution method. *If the equation is satisfied identically by making the substitutions $y = dy/dx = \cdots = d^n y/dx^n$ then $y = Ae^x$ is a solution.*

15.4 Exercises

15.1 A simple harmonic oscillator, of mass m and natural frequency ω_0, experiences an oscillating driving force $f(t) = ma\cos\omega t$. Therefore, its equation of motion is

$$\frac{d^2x}{dt^2} + \omega_0^2 x = a\cos\omega t,$$

where x is its position. Given that at $t = 0$ we have $x = dx/dt = 0$, find the function $x(t)$. Describe the solution if ω is approximately, but not exactly, equal to ω_0.

15.2 Find the roots of the auxiliary equation for the following. Hence solve them for the boundary conditions stated.

$$\text{(a)}\ \frac{d^2f}{dt^2} + 2\frac{df}{dt} + 5f = 0, \qquad \text{with } f(0) = 1, f'(0) = 0.$$

$$\text{(b)}\ \frac{d^2f}{dt^2} + 2\frac{df}{dt} + 5f = e^{-t}\cos 3t, \qquad \text{with } f(0) = 0, f'(0) = 0.$$

15.3 The theory of bent beams shows that at any point in the beam the ‘bending moment’ is given by K/ρ, where K is a constant (that depends upon the beam material and cross-sectional shape) and ρ is the radius of curvature at that point. Consider a light beam of length L whose ends, $x = 0$ and $x = L$, are supported at the same vertical height and which has a weight W suspended from its centre. Verify that at any point x ($0 \le x \le L/2$ for definiteness) the net magnitude of the bending moment (bending moment = force × perpendicular distance) due to the weight and support reactions, evaluated on either side of x, is $Wx/2$.

If the beam is only slightly bent, so that $(dy/dx)^2 \ll 1$, where $y = y(x)$ is the downward displacement of the beam at x, show that the beam profile satisfies the approximate equation

$$\frac{d^2y}{dx^2} = -\frac{Wx}{2K}.$$

By integrating this equation twice and using physically imposed conditions on your solution at $x = 0$ and $x = L/2$, show that the downward displacement at the centre of the beam is $WL^3/(48K)$.

15.4 Solve the differential equation

$$\frac{d^2f}{dt^2} + 6\frac{df}{dt} + 9f = e^{-t},$$

subject to the conditions $f = 0$ and $df/dt = \lambda$ at $t = 0$.

Find the equation satisfied by the positions of the turning points of $f(t)$ and hence, by drawing suitable sketch graphs, determine the number of turning points the solution has in the range $t > 0$ if (a) $\lambda = 1/4$, and (b) $\lambda = -1/4$.

15.5 The function $f(t)$ satisfies the differential equation

$$\frac{d^2f}{dt^2} + 8\frac{df}{dt} + 12f = 12e^{-4t}.$$

For the following sets of boundary conditions determine whether it has solutions, and, if so, find them:

(a) $f(0) = 0, \quad f'(0) = 0, \quad f(\ln\sqrt{2}) = 0;$
(b) $f(0) = 0, \quad f'(0) = -2, \quad f(\ln\sqrt{2}) = 0.$

15.6 Determine the values of α and β for which the following four functions are linearly dependent:

$$\begin{aligned} y_1(x) &= x\cosh x + \sinh x, \\ y_2(x) &= x\sinh x + \cosh x, \\ y_3(x) &= (x + \alpha)e^x, \\ y_4(x) &= (x + \beta)e^{-x}. \end{aligned}$$

You will find it convenient to work with those linear combinations of the $y_i(x)$ that can be written the most compactly.

15.7 A solution of the differential equation

$$\frac{d^2y}{dx^2} + 2\frac{dy}{dx} + y = 4e^{-x}$$

takes the value 1 when $x = 0$ and the value e^{-1} when $x = 1$. What is its value when $x = 2$?

15.8 The two functions $x(t)$ and $y(t)$ satisfy the simultaneous equations

$$\begin{aligned} \frac{dx}{dt} - 2y &= -\sin t, \\ \frac{dy}{dt} + 2x &= 5\cos t. \end{aligned}$$

Find explicit expressions for $x(t)$ and $y(t)$, given that $x(0) = 3$ and $y(0) = 2$. Sketch the solution trajectory in the xy-plane for $0 \le t < 2\pi$, showing that the trajectory crosses itself at $(0, 1/2)$ and passes through the points $(0, -3)$ and $(0, -1)$ in the negative x-direction.

15.9 Find the general solutions of

(a) $\dfrac{d^3y}{dx^3} - 12\dfrac{dy}{dx} + 16y = 32x - 8,$

(b) $\dfrac{d}{dx}\left(\dfrac{1}{y}\dfrac{dy}{dx}\right) + (2a\coth 2ax)\left(\dfrac{1}{y}\dfrac{dy}{dx}\right) = 2a^2,$

where a is a constant.

15.10 Use the method of Laplace transforms to solve

(a) $\dfrac{d^2f}{dt^2} + 5\dfrac{df}{dt} + 6f = 0, \qquad f(0) = 1,\ f'(0) = -4,$

(b) $\dfrac{d^2f}{dt^2} + 2\dfrac{df}{dt} + 5f = 0, \qquad f(0) = 1,\ f'(0) = 0.$

15.11 The quantities $x(t)$, $y(t)$ satisfy the simultaneous equations

$$\ddot{x} + 2n\dot{x} + n^2x = 0,$$
$$\ddot{y} + 2n\dot{y} + n^2y = \mu\dot{x},$$

where $x(0) = y(0) = \dot{y}(0) = 0$ and $\dot{x}(0) = \lambda$. Show that

$$y(t) = \tfrac{1}{2}\mu\lambda t^2\left(1 - \tfrac{1}{3}nt\right)\exp(-nt).$$

15.12 Use Laplace transforms to solve, for $t \geq 0$, the differential equations

$$\ddot{x} + 2x + y = \cos t,$$
$$\ddot{y} + 2x + 3y = 2\cos t,$$

which describe a coupled system that starts from rest at the equilibrium position. Show that the subsequent motion takes place along a straight line in the xy-plane. Verify that the frequency at which the system is driven is equal to one of the resonance frequencies of the system; explain why there is *no* resonant behaviour in the solution you have obtained.

15.13 Two unstable isotopes A and B and a stable isotope C have the following decay rates per atom present: $A \to B$, $3\ \mathrm{s}^{-1}$; $A \to C$, $1\ \mathrm{s}^{-1}$; $B \to C$, $2\ \mathrm{s}^{-1}$. Initially a quantity x_0 of A is present, but there are no atoms of the other two types. Using Laplace transforms, find the amount of C present at a later time t.

15.14 For a lightly damped ($\gamma < \omega_0$) harmonic oscillator driven at its undamped resonance frequency ω_0, the displacement $x(t)$ at time t satisfies the equation

$$\frac{d^2x}{dt^2} + 2\gamma\frac{dx}{dt} + \omega_0^2 x = F\sin\omega_0 t.$$

Use Laplace transforms to find the displacement at a general time if the oscillator starts from rest at its equilibrium position.

(a) Show that ultimately the oscillation has amplitude $F/(2\omega_0\gamma)$, with a phase lag of $\pi/2$ relative to the driving force per unit mass F.

(b) By differentiating the original equation, conclude that if $x(t)$ is expanded as a power series in t for small t, then the first non-vanishing term is $F\omega_0 t^3/6$. Confirm this conclusion by expanding your explicit solution.

15.15 The 'golden mean', which is said to describe the most aesthetically pleasing proportions for the sides of a rectangle (e.g. the ideal picture frame), is given by the limiting value of the ratio of successive terms of the Fibonacci series u_n, which is generated by

$$u_{n+2} = u_{n+1} + u_n,$$

with $u_0 = 0$ and $u_1 = 1$. Find an expression for the general term of the series and verify that the golden mean is equal to the larger root of the recurrence relation's characteristic equation.

15.16 In a particular scheme for numerically modelling one-dimensional fluid flow, the successive values, u_n, of the solution are connected for $n \geq 1$ by the difference equation

$$c(u_{n+1} - u_{n-1}) = d(u_{n+1} - 2u_n + u_{n-1}),$$

where c and d are positive constants. The boundary conditions are $u_0 = 0$ and $u_M = 1$. Find the solution to the equation, and show that successive values of u_n will have alternating signs if $c > d$.

15.17 The first few terms of a series u_n, starting with u_0, are $1, 2, 2, 1, 6, -3$. The series is generated by a recurrence relation of the form

$$u_n = Pu_{n-2} + Qu_{n-4},$$

where P and Q are constants. Find an expression for the general term of the series and show that, in fact, the series consists of two interleaved series given by

$$u_{2m} = \tfrac{2}{3} + \tfrac{1}{3}4^m,$$
$$u_{2m+1} = \tfrac{7}{3} - \tfrac{1}{3}4^m,$$

for $m = 0, 1, 2, \ldots$.

15.18 Find an explicit expression for the u_n satisfying

$$u_{n+1} + 5u_n + 6u_{n-1} = 2^n,$$

given that $u_0 = u_1 = 1$. Deduce that $2^n - 26(-3)^n$ is divisible by 5 for all non-negative integers n.

15.19 Find the general expression for the u_n satisfying

$$u_{n+1} = 2u_{n-2} - u_n$$

with $u_0 = u_1 = 0$ and $u_2 = 1$, and show that they can be written in the form

$$u_n = \frac{1}{5} - \frac{2^{n/2}}{\sqrt{5}} \cos\left(\frac{3\pi n}{4} - \phi\right),$$

where $\tan\phi = 2$.

15.20 Consider the seventh-order recurrence relation

$$u_{n+7} - u_{n+6} - u_{n+5} + u_{n+4} - u_{n+3} + u_{n+2} + u_{n+1} - u_n = 0.$$

Find the most general form of its solution, and show that:

(a) if only the four initial values $u_0 = 0$, $u_1 = 2$, $u_2 = 6$ and $u_3 = 12$, are specified, then the relation has one solution that cycles repeatedly through this set of four numbers;
(b) but if, in addition, it is required that $u_4 = 20$, $u_5 = 30$ and $u_6 = 42$ then the solution is unique, with $u_n = n(n + 1)$.

15.21 Find the general solution of

$$x^2\frac{d^2y}{dx^2} - x\frac{dy}{dx} + y = x,$$

given that $y(1) = 1$ and $y(e) = 2e$.

15.22 Find the general solution of

$$(x + 1)^2\frac{d^2y}{dx^2} + 3(x + 1)\frac{dy}{dx} + y = x^2.$$

15.23 Prove that the general solution of

$$(x-2)\frac{d^2y}{dx^2} + 3\frac{dy}{dx} + \frac{4y}{x^2} = 0$$

is given by

$$y(x) = \frac{1}{(x-2)^2}\left[k\left(\frac{2}{3x} - \frac{1}{2}\right) + cx^2\right].$$

15.24 Use the method of variation of parameters to find the general solutions of

(a) $\dfrac{d^2y}{dx^2} - y = x^n$, (b) $\dfrac{d^2y}{dx^2} - 2\dfrac{dy}{dx} + y = 2xe^x$.

15.25 Use the intermediate result of exercise 15.24(a) to find the Green's function that satisfies

$$\frac{d^2G(x,\xi)}{dx^2} - G(x,\xi) = \delta(x-\xi) \qquad \text{with} \qquad G(0,\xi) = G(1,\xi) = 0.$$

15.26 Consider the equation

$$F(x,y) = x(x+1)\frac{d^2y}{dx^2} + (2-x^2)\frac{dy}{dx} - (2+x)y = 0.$$

(a) Given that $y_1(x) = 1/x$ is one of its solutions, find a second linearly independent one,
 (i) by setting $y_2(x) = y_1(x)u(x)$, and
 (ii) by noting the sum of the coefficients in the equation.

(b) Hence, using the variation of parameters method, find the general solution of

$$F(x,y) = (x+1)^2.$$

15.27 Show generally that if $y_1(x)$ and $y_2(x)$ are linearly independent solutions of

$$\frac{d^2y}{dx^2} + p(x)\frac{dy}{dx} + q(x)y = 0,$$

with $y_1(0) = 0$ and $y_2(1) = 0$, then the Green's function $G(x,\xi)$ for the interval $0 \le x, \xi \le 1$ and with $G(0,\xi) = G(1,\xi) = 0$ can be written in the form

$$G(x,\xi) = \begin{cases} y_1(x)y_2(\xi)/W(\xi) & 0 < x < \xi, \\ y_2(x)y_1(\xi)/W(\xi) & \xi < x < 1, \end{cases}$$

where $W(x) = W[y_1(x), y_2(x)]$ is the Wronskian of $y_1(x)$ and $y_2(x)$.

15.28 Use the result of the previous exercise to find the Green's function $G(x,\xi)$ that satisfies

$$\frac{d^2G}{dx^2} + 3\frac{dG}{dx} + 2G = \delta(x-x),$$

in the interval $0 \le x, \xi \le 1$, with $G(0,\xi) = G(1,\xi) = 0$. Hence obtain integral expressions for the solution of

$$\frac{d^2y}{dx^2} + 3\frac{dy}{dx} + 2y = \begin{cases} 0 & 0 < x < x_0, \\ 1 & x_0 < x < 1, \end{cases}$$

distinguishing between the cases (a) $x < x_0$, and (b) $x > x_0$.

15.29 The equation of motion for a driven damped harmonic oscillator can be written

$$\ddot{x} + 2\dot{x} + (1 + \kappa^2)x = f(t),$$

with $\kappa \neq 0$. If it starts from rest with $x(0) = 0$ and $\dot{x}(0) = 0$, find the corresponding Green's function $G(t, \tau)$ and verify that it can be written as a function of $t - \tau$ only. Find the explicit solution when the driving force is the unit step function, i.e. $f(t) = H(t)$. Confirm your solution by taking the Laplace transforms of both it and the original equation.

15.30 Show that the Green's function for the equation

$$\frac{d^2y}{dx^2} + \frac{y}{4} = f(x),$$

subject to the boundary conditions $y(0) = y(\pi) = 0$, is given by

$$G(x, z) = \begin{cases} -2\cos\frac{1}{2}x \sin\frac{1}{2}z & 0 \leq z \leq x, \\ -2\sin\frac{1}{2}x \cos\frac{1}{2}z & x \leq z \leq \pi. \end{cases}$$

15.31 Find the Green's function $x = G(t, t_0)$ that solves

$$\frac{d^2x}{dt^2} + \alpha\frac{dx}{dt} = \delta(t - t_0)$$

under the initial conditions $x = dx/dt = 0$ at $t = 0$. Hence solve

$$\frac{d^2x}{dt^2} + \alpha\frac{dx}{dt} = f(t),$$

where $f(t) = 0$ for $t < 0$.
Evaluate your answer explicitly for $f(t) = Ae^{-at}$ $(t > 0)$.

15.32 Consider the equation

$$\frac{d^2y}{dx^2} + f(y) = 0,$$

where $f(y)$ can be any function.

(a) By multiplying through by dy/dx, obtain the general solution relating x and y.

(b) A mass m, initially at rest at the point $x = 0$, is accelerated by a force

$$f(x) = A(x_0 - x)\left[1 + 2\ln\left(1 - \frac{x}{x_0}\right)\right].$$

Its equation of motion is $m\,d^2x/dt^2 = f(x)$. Find x as a function of time, and show that ultimately the particle has travelled a distance x_0.

15.33 Solve

$$2y\frac{d^3y}{dx^3} + 2\left(y + 3\frac{dy}{dx}\right)\frac{d^2y}{dx^2} + 2\left(\frac{dy}{dx}\right)^2 = \sin x.$$

15.34 Find the general solution of the equation

$$x\frac{d^3y}{dx^3} + 2\frac{d^2y}{dx^2} = Ax.$$

15.35 Express the equation

$$\frac{d^2y}{dx^2} + 4x\frac{dy}{dx} + (4x^2 + 6)y = e^{-x^2}\sin 2x$$

in canonical form and hence find its general solution.

15.36 Find the form of the solutions of the equation

$$\frac{dy}{dx}\frac{d^3y}{dx^3} - 2\left(\frac{d^2y}{dx^2}\right)^2 + \left(\frac{dy}{dx}\right)^2 = 0$$

that have $y(0) = \infty$.

[You will need the result $\int^z \operatorname{cosech} u\, du = -\ln(\operatorname{cosech} z + \coth z)$.]

15.37 Consider the equation

$$x^p y'' + \frac{n+3-2p}{n-1} x^{p-1} y' + \left(\frac{p-2}{n-1}\right)^2 x^{p-2} y = y^n,$$

in which $p \neq 2$ and $n > -1$ but $n \neq 1$. For the boundary conditions $y(1) = 0$ and $y'(1) = \lambda$, show that the solution is $y(x) = v(x)x^{(p-2)/(n-1)}$, where $v(x)$ is given by

$$\int_0^{v(x)} \frac{dz}{\left[\lambda^2 + 2z^{n+1}/(n+1)\right]^{1/2}} = \ln x.$$

15.5 Hints and answers

15.1 The function is $a(\omega_0^2 - \omega^2)^{-1}(\cos\omega t - \cos\omega_0 t)$; for moderate t, $x(t)$ is a sine wave of linearly increasing amplitude $(t \sin\omega_0 t)/(2\omega_0)$; for large t it shows beats of maximum amplitude $2(\omega_0^2 - \omega^2)^{-1}$.

15.3 Ignore the term y'^2, compared with 1, in the expression for ρ. $y = 0$ at $x = 0$. From symmetry, $dy/dx = 0$ at $x = L/2$.

15.5 General solution $f(t) = Ae^{-6t} + Be^{-2t} - 3e^{-4t}$. (a) No solution, inconsistent boundary conditions; (b) $f(t) = 2e^{-6t} + e^{-2t} - 3e^{-4t}$.

15.7 The auxiliary equation has repeated roots and the RHS is contained in the complementary function. The solution is $y(x) = (A+Bx)e^{-x} + 2x^2e^{-x}$. $y(2) = 5e^{-2}$.

15.9 (a) The auxiliary equation has roots 2, 2, -4; $(A+Bx)\exp 2x + C\exp(-4x) + 2x + 1$; (b) multiply through by $\sinh 2ax$ and note that $\int \operatorname{cosech} 2ax\, dx = (2a)^{-1}\ln(|\tanh ax|)$; $y = B(\sinh 2ax)^{1/2}(|\tanh ax|)^A$.

15.11 Use Laplace transforms; write $s(s+n)^{-4}$ as $(s+n)^{-3} - n(s+n)^{-4}$.

15.13 $\mathcal{L}[C(t)] = x_0(s+8)/[s(s+2)(s+4)]$, yielding $C(t) = x_0[1 + \frac{1}{2}\exp(-4t) - \frac{3}{2}\exp(-2t)]$.

15.15 The characteristic equation is $\lambda^2 - \lambda - 1 = 0$. $u_n = [(1+\sqrt{5})^n - (1-\sqrt{5})^n]/(2^n\sqrt{5})$.

15.17 From u_4 and u_5, $P = 5, Q = -4$. $u_n = 3/2 - 5(-1)^n/6 + (-2)^n/4 + 2^n/12$.

15.19 The general solution is $A + B2^{n/2}\exp(i3\pi n/4) + C2^{n/2}\exp(i5\pi n/4)$. The initial values imply that $A = 1/5, B = (\sqrt{5}/10)\exp[i(\pi - \phi)]$ and $C = (\sqrt{5}/10)\exp[i(\pi + \phi)]$.

15.21 This is Euler's equation; setting $x = \exp t$ produces $d^2z/dt^2 - 2\,dz/dt + z = \exp t$, with complementary function $(A + Bt)\exp t$ and particular integral $t^2(\exp t)/2$; $y(x) = x + [x\ln x(1 + \ln x)]/2$.

15.23 After multiplication through by x^2 the coefficients are such that this is an exact equation. The resulting first-order equation, in standard form, needs an integrating factor $(x-2)^2/x^2$.

15.25 Given the boundary conditions, it is better to work with $\sinh x$ and $\sinh(1-x)$ than with $e^{\pm x}$; $G(x,\xi) = -[\sinh(1-\xi)\sinh x]/\sinh 1$ for $x < \xi$ and $-[\sinh(1-x)\sinh\xi]/\sinh 1$ for $x > \xi$.

15.27 Follow the method of subsection 15.2.5, but using general rather than specific functions.

15.29 $G(t,\tau) = 0$ for $t < \tau$ and $\kappa^{-1}e^{-(t-\tau)}\sin[\kappa(t-\tau)]$ for $t > \tau$. For a unit step input, $x(t) = (1+\kappa^2)^{-1}(1 - e^{-t}\cos\kappa t - \kappa^{-1}e^{-t}\sin\kappa t)$. Both transforms are equivalent to $s[(s+1)^2 + \kappa^2)]\bar{x} = 1$.

15.31 Use continuity and the step condition on $\partial G/\partial t$ at $t = t_0$ to show that $G(t, t_0) = \alpha^{-1}\{1 - \exp[\alpha(t_0 - t)]\}$ for $0 \le t_0 \le t$; $x(t) = A(\alpha - a)^{-1}\{a^{-1}[1 - \exp(-at)] - \alpha^{-1}[1 - \exp(-\alpha t)]\}$.

15.33 The LHS of the equation is exact for two stages of integration and then needs an integrating factor $\exp x$; $2y\, d^2y/dx^2 + 2y\, dy/dx + 2(dy/dx)^2$; $2y\, dy/dx + y^2 = d(y^2)/dx + y^2$; $y^2 = A\exp(-x) + Bx + C - (\sin x - \cos x)/2$.

15.35 Follow the method of subsection 15.2.6; $u(x) = e^{-x^2}$ and $v(x)$ satisfies $v'' + 4v = \sin 2x$, for which a particular integral is $(-x\cos 2x)/4$. The general solution is $y(x) = [A\sin 2x + (B - \frac{1}{4}x)\cos 2x]e^{-x^2}$.

15.37 The equation is isobaric, with y of weight m, where $m + p - 2 = mn$; $v(x)$ satisfies $x^2v'' + xv' = v^n$. Set $x = e^t$ and $v(x) = u(t)$, leading to $u'' = u^n$ with $u(0) = 0, u'(0) = \lambda$. Multiply both sides by u' to make the equation exact.

16

Series solutions of ordinary differential equations

In the previous chapter the solution of both homogeneous and non-homogeneous linear ordinary differential equations (ODEs) of order ≥ 2 was discussed. In particular we developed methods for solving some equations in which the coefficients were not constant but functions of the independent variable x. In each case we were able to write the solutions to such equations in terms of elementary functions, or as integrals. In general, however, the solutions of equations with variable coefficients cannot be written in this way, and we must consider alternative approaches.

In this chapter we discuss a method for obtaining solutions to linear ODEs in the form of convergent series. Such series can be evaluated numerically, and those occurring most commonly are named and tabulated. There is in fact no distinct borderline between this and the previous chapter, since solutions in terms of elementary functions may equally well be written as convergent series (i.e. the relevant Taylor series). Indeed, it is partly because some series occur so frequently that they are given special names such as $\sin x$, $\cos x$ or $\exp x$.

Since we shall be concerned principally with second-order linear ODEs in this chapter, we begin with a discussion of these equations, and obtain some general results that will prove useful when we come to discuss series solutions.

16.1 Second-order linear ordinary differential equations

Any homogeneous second-order linear ODE can be written in the form

$$y'' + p(x)y' + q(x)y = 0, \tag{16.1}$$

where $y' = dy/dx$ and $p(x)$ and $q(x)$ are given functions of x. From the previous chapter, we recall that the most general form of the solution to (16.1) is

$$y(x) = c_1 y_1(x) + c_2 y_2(x), \tag{16.2}$$

where $y_1(x)$ and $y_2(x)$ are *linearly independent* solutions of (16.1), and c_1 and c_2 are constants that are fixed by the boundary conditions (if supplied).

A full discussion of the linear independence of sets of functions was given at the beginning of the previous chapter, but for just two functions y_1 and y_2 to be linearly independent we simply require that y_2 is not a multiple of y_1. Equivalently, y_1 and y_2 must be such that the equation

$$c_1y_1(x) + c_2y_2(x) = 0$$

is *only* satisfied for $c_1 = c_2 = 0$. Therefore the linear independence of $y_1(x)$ and $y_2(x)$ can usually be deduced by inspection but in any case can always be verified by the evaluation of the Wronskian of the two solutions,

$$W(x) = \begin{vmatrix} y_1 & y_2 \\ y_1' & y_2' \end{vmatrix} = y_1y_2' - y_2y_1'. \tag{16.3}$$

If $W(x) \neq 0$ anywhere in a given interval then y_1 and y_2 are linearly independent in that interval.

An alternative expression for $W(x)$, of which we will make use later, may be derived by differentiating (16.3) with respect to x to give

$$W' = y_1y_2'' + y_1'y_2' - y_2y_1'' - y_2'y_1' = y_1y_2'' - y_1''y_2.$$

Since both y_1 and y_2 satisfy (16.1), we may substitute for y_1'' and y_2'' to obtain

$$W' = -y_1(py_2' + qy_2) + (py_1' + qy_1)y_2 = -p(y_1y_2' - y_1'y_2) = -pW.$$

Integrating, we find

$$W(x) = C\exp\left\{-\int^x p(u)\,du\right\}, \tag{16.4}$$

where C is a constant. We note further that in the special case $p(x) \equiv 0$ we obtain $W = $ constant.

►*The functions $y_1 = \sin x$ and $y_2 = \cos x$ are both solutions of the equation $y'' + y = 0$. Evaluate the Wronskian of these two solutions, and hence show that they are linearly independent.*

The Wronskian of y_1 and y_2 is given by

$$W = y_1y_2' - y_2y_1' = -\sin^2 x - \cos^2 x = -1.$$

Since $W \neq 0$ the two solutions are linearly independent. We also note that $y'' + y = 0$ is a special case of (16.1) with $p(x) = 0$. We therefore expect, from (16.4), that W will be a constant, as is indeed the case. ◄

From the previous chapter we recall that, once we have obtained the general solution to the homogeneous second-order ODE (16.1) in the form (16.2), the general solution to the *inhomogeneous* equation

$$y'' + p(x)y' + q(x)y = f(x) \tag{16.5}$$

can be written as the sum of the solution to the homogeneous equation $y_c(x)$ (the complementary function) and *any* function $y_p(x)$ (the particular integral) that satisfies (16.5) and is linearly independent of $y_c(x)$. We have therefore

$$y(x) = c_1 y_1(x) + c_2 y_2(x) + y_p(x). \tag{16.6}$$

General methods for obtaining y_p, that are applicable to equations with variable coefficients, such as the variation of parameters or Green's functions, were discussed in the previous chapter. An alternative description of the Green's function method for solving inhomogeneous equations is given in the next chapter. For the present, however, we will restrict our attention to the solutions of homogeneous ODEs in the form of convergent series.

16.1.1 Ordinary and singular points of an ODE

So far we have implicitly assumed that $y(x)$ is a *real* function of a *real* variable x. However, this is not always the case, and in the remainder of this chapter we broaden our discussion by generalising to a *complex* function $y(z)$ of a *complex* variable z.

Let us therefore consider the second-order linear homogeneous ODE

$$y'' + p(z)y' + q(z) = 0, \tag{16.7}$$

where now $y' = dy/dz$; this is a straightforward generalisation of (16.1). A full discussion of complex functions and differentiation with respect to a complex variable z is given in chapter 24, but for the purposes of the present chapter we need not concern ourselves with many of the subtleties that exist. In particular, we may treat differentiation with respect to z in a way analogous to ordinary differentiation with respect to a real variable x.

In (16.7), if, at some point $z = z_0$, the functions $p(z)$ and $q(z)$ are finite and can be expressed as complex power series (see section 4.5), i.e.

$$p(z) = \sum_{n=0}^{\infty} p_n (z - z_0)^n, \qquad q(z) = \sum_{n=0}^{\infty} q_n (z - z_0)^n,$$

then $p(z)$ and $q(z)$ are said to be *analytic* at $z = z_0$, and this point is called an *ordinary point* of the ODE. If, however, $p(z)$ or $q(z)$, or both, diverge at $z = z_0$ then it is called a *singular point* of the ODE.

Even if an ODE is singular at a given point $z = z_0$, it may still possess a non-singular (finite) solution at that point. In fact the necessary and sufficient condition[§] for such a solution to exist is that $(z - z_0)p(z)$ and $(z - z_0)^2 q(z)$ are both analytic at $z = z_0$. Singular points that have this property are called *regular*

[§] See, for example, H. Jeffreys and B. S. Jeffreys, *Methods of Mathematical Physics*, 3rd edn (Cambridge: Cambridge University Press, 1966), p. 479.

singular points, whereas any singular point not satisfying both these criteria is termed an *irregular* or *essential* singularity.

►*Legendre's equation has the form*

$$(1-z^2)y'' - 2zy' + \ell(\ell+1)y = 0, \tag{16.8}$$

where ℓ is a constant. Show that $z = 0$ is an ordinary point and $z = \pm 1$ are regular singular points of this equation.

Firstly, divide through by $1 - z^2$ to put the equation into our standard form (16.7):

$$y'' - \frac{2z}{1-z^2}y' + \frac{\ell(\ell+1)}{1-z^2}y = 0.$$

Comparing this with (16.7), we identify $p(z)$ and $q(z)$ as

$$p(z) = \frac{-2z}{1-z^2} = \frac{-2z}{(1+z)(1-z)}, \qquad q(z) = \frac{\ell(\ell+1)}{1-z^2} = \frac{\ell(\ell+1)}{(1+z)(1-z)}.$$

By inspection, $p(z)$ and $q(z)$ are analytic at $z = 0$, which is therefore an ordinary point, but both diverge for $z = \pm 1$, which are thus singular points. However, at $z = 1$ we see that both $(z-1)p(z)$ and $(z-1)^2 q(z)$ are analytic and hence $z = 1$ is a regular singular point. Similarly, at $z = -1$ both $(z+1)p(z)$ and $(z+1)^2 q(z)$ are analytic, and it too is a regular singular point. ◄

So far we have assumed that z_0 is finite. However, we may sometimes wish to determine the nature of the point $|z| \to \infty$. This may be achieved straightforwardly by substituting $w = 1/z$ into the equation and investigating the behaviour at $w = 0$.

►*Show that Legendre's equation has a regular singularity at $|z| \to \infty$.*

Letting $w = 1/z$, the derivatives with respect to z become

$$\frac{dy}{dz} = \frac{dy}{dw}\frac{dw}{dz} = -\frac{1}{z^2}\frac{dy}{dw} = -w^2\frac{dy}{dw},$$

$$\frac{d^2y}{dz^2} = \frac{dw}{dz}\frac{d}{dw}\left(\frac{dy}{dz}\right) = -w^2\left(-2w\frac{dy}{dw} - w^2\frac{d^2y}{dw^2}\right) = w^3\left(2\frac{dy}{dw} + w\frac{d^2y}{dw^2}\right).$$

If we substitute these derivatives into Legendre's equation (16.8) we obtain

$$\left(1 - \frac{1}{w^2}\right)w^3\left(2\frac{dy}{dw} + w\frac{d^2y}{dw^2}\right) + 2\frac{1}{w}w^2\frac{dy}{dw} + \ell(\ell+1)y = 0,$$

which simplifies to give

$$w^2(w^2-1)\frac{d^2y}{dw^2} + 2w^3\frac{dy}{dw} + \ell(\ell+1)y = 0.$$

Dividing through by $w^2(w^2-1)$ to put the equation into standard form, and comparing with (16.7), we identify $p(w)$ and $q(w)$ as

$$p(w) = \frac{2w}{w^2-1}, \qquad q(w) = \frac{\ell(\ell+1)}{w^2(w^2-1)}.$$

At $w = 0$, $p(w)$ is analytic but $q(w)$ diverges, and so the point $|z| \to \infty$ is a singular point of Legendre's equation. However, since wp and w^2q are both analytic at $w = 0$, $|z| \to \infty$ is a regular singular point. ◄

Equation	Regular singularities	Essential singularities
Hypergeometric $z(1-z)y'' + [c-(a+b+1)z]y' - aby = 0$	$0, 1, \infty$	—
Legendre $(1-z^2)y'' - 2zy' + \ell(\ell+1)y = 0$	$-1, 1, \infty$	—
Associated Legendre $(1-z^2)y'' - 2zy' + \left[\ell(\ell+1) - \frac{m^2}{1-z^2}\right]y = 0$	$-1, 1, \infty$	—
Chebyshev $(1-z^2)y'' - zy' + \nu^2 y = 0$	$-1, 1, \infty$	—
Confluent hypergeometric $zy'' + (c-z)y' - ay = 0$	0	∞
Bessel $z^2y'' + zy' + (z^2-\nu^2)y = 0$	0	∞
Laguerre $zy'' + (1-z)y' + \nu y = 0$	0	∞
Associated Laguerre $zy'' + (m+1-z)y' + (\nu-m)y = 0$	0	∞
Hermite $y'' - 2zy' + 2\nu y = 0$	—	∞
Simple harmonic oscillator $y'' + \omega^2 y = 0$	—	∞

Table 16.1 Important second-order linear ODEs in the physical sciences and engineering.

Table 16.1 lists the singular points of several second-order linear ODEs that play important roles in the analysis of many problems in physics and engineering. A full discussion of the solutions to each of the equations in table 16.1 and their properties is left until chapter 18. We now discuss the general methods by which series solutions may be obtained.

16.2 Series solutions about an ordinary point

If $z = z_0$ is an ordinary point of (16.7) then it may be shown that *every* solution $y(z)$ of the equation is also analytic at $z = z_0$. From now on we will take z_0 as the origin, i.e. $z_0 = 0$. If this is not already the case, then a substitution $Z = z - z_0$ will make it so. Since every solution is analytic, $y(z)$ can be represented by a power series of the form (see section 24.11)

$$y(z) = \sum_{n=0}^{\infty} a_n z^n. \tag{16.9}$$

Moreover, it may be shown that such a power series converges for $|z| < R$, where R is the radius of convergence and is equal to the distance from $z = 0$ to the nearest singular point of the ODE (see chapter 24). At the radius of convergence, however, the series may or may not converge (as shown in section 4.5).

Since every solution of (16.7) is analytic at an ordinary point, it is always possible to obtain two *independent* solutions (from which the general solution (16.2) can be constructed) of the form (16.9). The derivatives of y with respect to z are given by

$$y' = \sum_{n=0}^{\infty} n a_n z^{n-1} = \sum_{n=0}^{\infty} (n+1) a_{n+1} z^n, \tag{16.10}$$

$$y'' = \sum_{n=0}^{\infty} n(n-1) a_n z^{n-2} = \sum_{n=0}^{\infty} (n+2)(n+1) a_{n+2} z^n. \tag{16.11}$$

Note that, in each case, in the first equality the sum can still start at $n = 0$ since the first term in (16.10) and the first two terms in (16.11) are automatically zero. The second equality in each case is obtained by shifting the summation index so that the sum can be written in terms of coefficients of z^n. By substituting (16.9)–(16.11) into the ODE (16.7), and requiring that the coefficients of each power of z sum to zero, we obtain a *recurrence relation* expressing each a_n in terms of the previous a_r $(0 \leq r \leq n-1)$.

► *Find the series solutions, about $z = 0$, of*

$$y'' + y = 0.$$

By inspection, $z = 0$ is an ordinary point of the equation, and so we may obtain two independent solutions by making the substitution $y = \sum_{n=0}^{\infty} a_n z^n$. Using (16.9) and (16.11) we find

$$\sum_{n=0}^{\infty} (n+2)(n+1) a_{n+2} z^n + \sum_{n=0}^{\infty} a_n z^n = 0,$$

which may be written as

$$\sum_{n=0}^{\infty} [(n+2)(n+1) a_{n+2} + a_n] z^n = 0.$$

For this equation to be satisfied we require that the coefficient of each power of z vanishes *separately*, and so we obtain the two-term recurrence relation

$$a_{n+2} = -\frac{a_n}{(n+2)(n+1)} \qquad \text{for } n \geq 0.$$

Using this relation, we can calculate, say, the even coefficients a_2, a_4, a_6 and so on, for a given a_0. Alternatively, starting with a_1, we obtain the odd coefficients a_3, a_5, etc. Two independent solutions of the ODE can be obtained by setting either $a_0 = 0$ or $a_1 = 0$. Firstly, if we set $a_1 = 0$ and choose $a_0 = 1$ then we obtain the solution

$$y_1(z) = 1 - \frac{z^2}{2!} + \frac{z^4}{4!} - \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} z^{2n}.$$

Secondly, if we set $a_0 = 0$ and choose $a_1 = 1$ then we obtain a second, *independent*, solution

$$y_2(z) = z - \frac{z^3}{3!} + \frac{z^5}{5!} - \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} z^{2n+1}.$$

Recognising these two series as $\cos z$ and $\sin z$, we can write the general solution as

$$y(z) = c_1 \cos z + c_2 \sin z,$$

where c_1 and c_2 are arbitrary constants that are fixed by boundary conditions (if supplied). We note that both solutions converge for all z, as might be expected since the ODE possesses no singular points (except $|z| \to \infty$). ◄

Solving the above example was quite straightforward and the resulting series were easily recognised and written in *closed form* (i.e. in terms of elementary functions); *this is not usually the case*. Another simplifying feature of the previous example was that we obtained a two-term recurrence relation relating a_{n+2} and a_n, so that the odd- and even-numbered coefficients were independent of one another. In general, the recurrence relation expresses a_n in terms of any number of the previous a_r $(0 \le r \le n-1)$.

►*Find the series solutions, about $z = 0$, of*

$$y'' - \frac{2}{(1-z)^2} y = 0.$$

By inspection, $z = 0$ is an ordinary point, and therefore we may find two independent solutions by substituting $y = \sum_{n=0}^{\infty} a_n z^n$. Using (16.10) and (16.11), and multiplying through by $(1-z)^2$, we find

$$(1 - 2z + z^2) \sum_{n=0}^{\infty} n(n-1) a_n z^{n-2} - 2 \sum_{n=0}^{\infty} a_n z^n = 0,$$

which leads to

$$\sum_{n=0}^{\infty} n(n-1) a_n z^{n-2} - 2 \sum_{n=0}^{\infty} n(n-1) a_n z^{n-1} + \sum_{n=0}^{\infty} n(n-1) a_n z^n - 2 \sum_{n=0}^{\infty} a_n z^n = 0.$$

In order to write all these series in terms of the coefficients of z^n, we must shift the summation index in the first two sums, obtaining

$$\sum_{n=0}^{\infty} (n+2)(n+1) a_{n+2} z^n - 2 \sum_{n=0}^{\infty} (n+1) n a_{n+1} z^n + \sum_{n=0}^{\infty} (n^2 - n - 2) a_n z^n = 0,$$

which can be written as

$$\sum_{n=0}^{\infty} (n+1)[(n+2) a_{n+2} - 2n a_{n+1} + (n-2) a_n] z^n = 0.$$

By demanding that the coefficients of each power of z vanish separately, we obtain the three-term recurrence relation

$$(n+2)a_{n+2} - 2na_{n+1} + (n-2)a_n = 0 \qquad \text{for } n \geq 0,$$

which determines a_n for $n \geq 2$ in terms of a_0 and a_1. Three-term (or more) recurrence relations are a nuisance and, in general, can be difficult to solve. This particular recurrence relation, however, has two straightforward solutions. One solution is $a_n = a_0$ for all n, in which case (choosing $a_0 = 1$) we find

$$y_1(z) = 1 + z + z^2 + z^3 + \cdots = \frac{1}{1-z}.$$

The other solution to the recurrence relation is $a_1 = -2a_0$, $a_2 = a_0$ and $a_n = 0$ for $n > 2$, so that (again choosing $a_0 = 1$) we obtain a *polynomial* solution to the ODE:

$$y_2(z) = 1 - 2z + z^2 = (1-z)^2.$$

The linear independence of y_1 and y_2 is obvious but can be checked by computing the Wronskian

$$W = y_1 y_2' - y_1' y_2 = \frac{1}{1-z}[-2(1-z)] - \frac{1}{(1-z)^2}(1-z)^2 = -3.$$

Since $W \neq 0$, the two solutions y_1 and y_2 are indeed linearly independent. The general solution of the ODE is therefore

$$y(z) = \frac{c_1}{1-z} + c_2(1-z)^2.$$

We observe that y_1 (and hence the general solution) is singular at $z = 1$, which is the singular point of the ODE nearest to $z = 0$, but the polynomial solution, y_2, is valid for all finite z. ◄

The above example illustrates the possibility that, in some cases, we may find that the recurrence relation leads to $a_n = 0$ for $n > N$, for one or both of the two solutions; we then obtain a *polynomial* solution to the equation. Polynomial solutions are discussed more fully in section 16.5, but one obvious property of such solutions is that they converge for all finite z. By contrast, as mentioned above, for solutions in the form of an infinite series the circle of convergence extends only as far as the singular point nearest to that about which the solution is being obtained.

16.3 Series solutions about a regular singular point

From table 16.1 we see that several of the most important second-order linear ODEs in physics and engineering have regular singular points in the finite complex plane. We must extend our discussion, therefore, to obtaining series solutions to ODEs about such points. In what follows we assume that the regular singular point about which the solution is required is at $z = 0$, since, as we have seen, if this is not already the case then a substitution of the form $Z = z - z_0$ will make it so.

If $z = 0$ is a regular singular point of the equation

$$y'' + p(z)y' + q(z)y = 0$$

then at least one of $p(z)$ and $q(z)$ is not analytic at $z = 0$, and in general we should not expect to find a power series solution of the form (16.9). We must therefore extend the method to include a more general form for the solution. In fact, it may be shown (Fuch's theorem) that there exists *at least one* solution to the above equation, of the form

$$y = z^{\sigma} \sum_{n=0}^{\infty} a_n z^n, \tag{16.12}$$

where the exponent σ is a number that may be real or complex and where $a_0 \neq 0$ (since, if it were otherwise, σ could be redefined as $\sigma + 1$ or $\sigma + 2$ or $\cdots$ so as to make $a_0 \neq 0$). Such a series is called a generalised power series or *Frobenius series*. As in the case of a simple power series solution, the radius of convergence of the Frobenius series is, in general, equal to the distance to the nearest singularity of the ODE.

Since $z = 0$ is a regular singularity of the ODE, it follows that $zp(z)$ and $z^2q(z)$ are analytic at $z = 0$, so that we may write

$$zp(z) \equiv s(z) = \sum_{n=0}^{\infty} s_n z^n,$$
$$z^2q(z) \equiv t(z) = \sum_{n=0}^{\infty} t_n z^n,$$

where we have defined the analytic functions $s(z)$ and $t(z)$ for later convenience. The original ODE therefore becomes

$$y'' + \frac{s(z)}{z}y' + \frac{t(z)}{z^2}y = 0.$$

Let us substitute the Frobenius series (16.12) into this equation. The derivatives of (16.12) with respect to z are given by

$$y' = \sum_{n=0}^{\infty}(n+\sigma)a_n z^{n+\sigma-1}, \tag{16.13}$$

$$y'' = \sum_{n=0}^{\infty}(n+\sigma)(n+\sigma-1)a_n z^{n+\sigma-2}, \tag{16.14}$$

and we obtain

$$\sum_{n=0}^{\infty}(n+\sigma)(n+\sigma-1)a_n z^{n+\sigma-2} + s(z)\sum_{n=0}^{\infty}(n+\sigma)a_n z^{n+\sigma-2} + t(z)\sum_{n=0}^{\infty} a_n z^{n+\sigma-2} = 0.$$

Dividing this equation through by $z^{\sigma-2}$, we find

$$\sum_{n=0}^{\infty}\left[(n+\sigma)(n+\sigma-1) + s(z)(n+\sigma) + t(z)\right] a_n z^n = 0. \tag{16.15}$$

Setting $z = 0$, all terms in the sum with $n > 0$ vanish, implying that

$$[\sigma(\sigma - 1) + s(0)\sigma + t(0)]a_0 = 0,$$

which, since we require $a_0 \neq 0$, yields the *indicial equation*

$$\sigma(\sigma - 1) + s(0)\sigma + t(0) = 0. \tag{16.16}$$

This equation is a quadratic in σ and in general has two roots, the nature of which determines the forms of possible series solutions.

The two roots of the indicial equation, σ_1 and σ_2, are called the *indices* of the regular singular point. By substituting each of these roots into (16.15) in turn and requiring that the coefficients of each power of z vanish separately, we obtain a recurrence relation (for each root) expressing each a_n as a function of the previous a_r $(0 \leq r \leq n - 1)$. We will see that the larger root of the indicial equation always yields a solution to the ODE in the form of a Frobenius series (16.12). The form of the second solution depends, however, on the relationship between the two indices σ_1 and σ_2. There are three possible general cases: (i) distinct roots not differing by an integer; (ii) repeated roots; (iii) distinct roots differing by an integer (not equal to zero). Below, we discuss each of these in turn.

Before continuing, however, we note that, as was the case for solutions in the form of a simple power series, it is always worth investigating whether a Frobenius series found as a solution to a problem is summable in closed form or expressible in terms of known functions. We illustrate this point below, but the reader should avoid gaining the impression that this is always so or that, if one worked hard enough, a closed-form solution could always be found without using the series method. As mentioned earlier, this is *not* the case, and very often an infinite series solution is the best one can do.

16.3.1 Distinct roots not differing by an integer

If the roots of the indicial equation, σ_1 and σ_2, differ by an amount that is not an integer then the recurrence relations corresponding to each root lead to two linearly independent solutions of the ODE:

$$y_1(z) = z^{\sigma_1} \sum_{n=0}^{\infty} a_n z^n, \qquad y_2(z) = z^{\sigma_2} \sum_{n=0}^{\infty} b_n z^n,$$

with both solutions taking the form of a Frobenius series. The linear independence of these two solutions follows from the fact that y_2/y_1 is not a constant since $\sigma_1 - \sigma_2$ is not an integer. Because y_1 and y_2 are linearly independent, we may use them to construct the general solution $y = c_1 y_1 + c_2 y_2$.

We also note that this case includes complex conjugate roots where $\sigma_2 = \sigma_1^*$, since $\sigma_1 - \sigma_2 = \sigma_1 - \sigma_1^* = 2i \operatorname{Im} \sigma_1$ cannot be equal to a real integer.

►*Find the power series solutions about $z = 0$ of*

$$4zy'' + 2y' + y = 0.$$

Dividing through by $4z$ to put the equation into standard form, we obtain

$$y'' + \frac{1}{2z}y' + \frac{1}{4z}y = 0, \tag{16.17}$$

and on comparing with (16.7) we identify $p(z) = 1/(2z)$ and $q(z) = 1/(4z)$. Clearly $z = 0$ is a singular point of (16.17), but since $zp(z) = 1/2$ and $z^2q(z) = z/4$ are finite there, it is a regular singular point. We therefore substitute the Frobenius series $y = z^\sigma \sum_{n=0}^{\infty} a_n z^n$ into (16.17). Using (16.13) and (16.14), we obtain

$$\sum_{n=0}^{\infty}(n+\sigma)(n+\sigma-1)a_n z^{n+\sigma-2} + \frac{1}{2z}\sum_{n=0}^{\infty}(n+\sigma)a_n z^{n+\sigma-1} + \frac{1}{4z}\sum_{n=0}^{\infty} a_n z^{n+\sigma} = 0,$$

which, on dividing through by $z^{\sigma-2}$, gives

$$\sum_{n=0}^{\infty}\left[(n+\sigma)(n+\sigma-1) + \tfrac{1}{2}(n+\sigma) + \tfrac{1}{4}z\right] a_n z^n = 0. \tag{16.18}$$

If we set $z = 0$ then all terms in the sum with $n > 0$ vanish, and we obtain the indicial equation

$$\sigma(\sigma-1) + \tfrac{1}{2}\sigma = 0,$$

which has roots $\sigma = 1/2$ and $\sigma = 0$. Since these roots do not differ by an integer, we expect to find two independent solutions to (16.17), in the form of Frobenius series.

Demanding that the coefficients of z^n vanish separately in (16.18), we obtain the recurrence relation

$$(n+\sigma)(n+\sigma-1)a_n + \tfrac{1}{2}(n+\sigma)a_n + \tfrac{1}{4}a_{n-1} = 0. \tag{16.19}$$

If we choose the larger root, $\sigma = 1/2$, of the indicial equation then (16.19) becomes

$$(4n^2 + 2n)a_n + a_{n-1} = 0 \qquad \Rightarrow \qquad a_n = \frac{-a_{n-1}}{2n(2n+1)}.$$

Setting $a_0 = 1$, we find $a_n = (-1)^n/(2n+1)!$, and so the solution to (16.17) is given by

$$\begin{aligned} y_1(z) &= \sqrt{z}\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)!}z^n \\ &= \sqrt{z} - \frac{(\sqrt{z})^3}{3!} + \frac{(\sqrt{z})^5}{5!} - \cdots = \sin\sqrt{z}. \end{aligned}$$

To obtain the second solution we set $\sigma = 0$ (the smaller root of the indicial equation) in (16.19), which gives

$$(4n^2 - 2n)a_n + a_{n-1} = 0 \qquad \Rightarrow \qquad a_n = -\frac{a_{n-1}}{2n(2n-1)}.$$

Setting $a_0 = 1$ now gives $a_n = (-1)^n/(2n)!$, and so the second (independent) solution to (16.17) is

$$y_2(z) = \sum_{n=0}^{\infty}\frac{(-1)^n}{(2n)!}z^n = 1 - \frac{(\sqrt{z})^2}{2!} + \frac{(\sqrt{4})^4}{4!} - \cdots = \cos\sqrt{z}.$$

We may check that $y_1(z)$ and $y_2(z)$ are indeed linearly independent by computing the Wronskian as follows:

$$\begin{aligned} W &= y_1 y_2' - y_2 y_1' \\ &= \sin\sqrt{z}\left(-\frac{1}{2\sqrt{z}}\sin\sqrt{z}\right) - \cos\sqrt{z}\left(\frac{1}{2\sqrt{z}}\cos\sqrt{z}\right) \\ &= -\frac{1}{2\sqrt{z}}\left(\sin^2\sqrt{z} + \cos^2\sqrt{z}\right) = -\frac{1}{2\sqrt{z}} \neq 0. \end{aligned}$$

Since $W \neq 0$, the solutions $y_1(z)$ and $y_2(z)$ are linearly independent. Hence, the general solution to (16.17) is given by

$$y(z) = c_1 \sin\sqrt{z} + c_2 \cos\sqrt{z}. \blacktriangleleft$$

16.3.2 Repeated root of the indicial equation

If the indicial equation has a repeated root, so that $\sigma_1 = \sigma_2 = \sigma$, then obviously only one solution in the form of a Frobenius series (16.12) may be found as described above, i.e.

$$y_1(z) = z^\sigma \sum_{n=0}^{\infty} a_n z^n.$$

Methods for obtaining a second, linearly independent, solution are discussed in section 16.4.

16.3.3 Distinct roots differing by an integer

Whatever the roots of the indicial equation, the recurrence relation corresponding to the larger of the two always leads to a solution of the ODE. However, if the roots of the indicial equation differ by an integer then the recurrence relation corresponding to the smaller root may or may not lead to a second linearly independent solution, depending on the ODE under consideration. Note that for complex roots of the indicial equation, the 'larger' root is taken to be the one with the larger real part.

►*Find the power series solutions about $z = 0$ of*

$$z(z-1)y'' + 3zy' + y = 0. \tag{16.20}$$

Dividing through by $z(z-1)$ to put the equation into standard form, we obtain

$$y'' + \frac{3}{(z-1)}y' + \frac{1}{z(z-1)}y = 0, \tag{16.21}$$

and on comparing with (16.7) we identify $p(z) = 3/(z-1)$ and $q(z) = 1/[z(z-1)]$. We immediately see that $z = 0$ is a singular point of (16.21), but since $zp(z) = 3z/(z-1)$ and $z^2 q(z) = z/(z-1)$ are finite there, it is a regular singular point and we expect to find at least one solution in the form of a Frobenius series. We therefore substitute $y = z^\sigma \sum_{n=0}^{\infty} a_n z^n$ into (16.21) and, using (16.13) and (16.14), we obtain

$$\sum_{n=0}^{\infty}(n+\sigma)(n+\sigma-1)a_n z^{n+\sigma-2} + \frac{3}{z-1}\sum_{n=0}^{\infty}(n+\sigma)a_n z^{n+\sigma-1} + \frac{1}{z(z-1)}\sum_{n=0}^{\infty} a_n z^{n+\sigma} = 0,$$

which, on dividing through by $z^{\sigma-2}$, gives

$$\sum_{n=0}^{\infty}\left[(n+\sigma)(n+\sigma-1) + \frac{3z}{z-1}(n+\sigma) + \frac{z}{z-1}\right] a_n z^n = 0.$$

Although we could use this expression to find the indicial equation and recurrence relations, the working is simpler if we now multiply through by $z-1$ to give

$$\sum_{n=0}^{\infty}\left[(z-1)(n+\sigma)(n+\sigma-1) + 3z(n+\sigma) + z\right] a_n z^n = 0. \tag{16.22}$$

If we set $z = 0$ then all terms in the sum with the exponent of z greater than zero vanish, and we obtain the indicial equation

$$\sigma(\sigma-1) = 0,$$

which has the roots $\sigma = 1$ and $\sigma = 0$. Since the roots differ by an integer (unity), it may not be possible to find two linearly independent solutions of (16.21) in the form of Frobenius series. We are guaranteed, however, to find one such solution corresponding to the larger root, $\sigma = 1$.

Demanding that the coefficients of z^n vanish separately in (16.22), we obtain the recurrence relation

$$(n-1+\sigma)(n-2+\sigma)a_{n-1} - (n+\sigma)(n+\sigma-1)a_n + 3(n-1+\sigma)a_{n-1} + a_{n-1} = 0,$$

which can be simplified to give

$$(n+\sigma-1)a_n = (n+\sigma)a_{n-1}. \tag{16.23}$$

On substituting $\sigma = 1$ into this expression, we obtain

$$a_n = \left(\frac{n+1}{n}\right) a_{n-1},$$

and on setting $a_0 = 1$ we find $a_n = n+1$; so one solution to (16.21) is given by

$$y_1(z) = z\sum_{n=0}^{\infty}(n+1)z^n = z(1+2z+3z^2+\cdots)$$
$$= \frac{z}{(1-z)^2}. \tag{16.24}$$

If we attempt to find a second solution (corresponding to the smaller root of the indicial equation) by setting $\sigma = 0$ in (16.23), we find

$$a_n = \left(\frac{n}{n-1}\right) a_{n-1}.$$

But we require $a_0 \neq 0$, so a_1 is formally infinite and the method fails. We discuss how to find a second linearly independent solution in the next section. ◀

One particular case is worth mentioning. If the point about which the solution is required, i.e. $z = 0$, is in fact an ordinary point of the ODE rather than a regular singular point, then substitution of the Frobenius series (16.12) leads to an indicial equation with roots $\sigma = 0$ and $\sigma = 1$. Although these roots differ by an integer (unity), the recurrence relations corresponding to the two roots yield two linearly independent power series solutions (one for each root), as expected from section 16.2.

16.4 Obtaining a second solution

Whilst attempting to construct solutions to an ODE in the form of Frobenius series about a regular singular point, we found in the previous section that when the indicial equation has a repeated root, or roots differing by an integer, we can (in general) find only one solution of this form. In order to construct the general solution to the ODE, however, we require two linearly independent solutions y_1 and y_2. We now consider several methods for obtaining a second solution in this case.

16.4.1 The Wronskian method

If y_1 and y_2 are two linearly independent solutions of the standard equation

$$y'' + p(z)y' + q(z)y = 0$$

then the Wronskian of these two solutions is given by $W(z) = y_1y_2' - y_2y_1'$. Dividing the Wronskian by y_1^2 we obtain

$$\frac{W}{y_1^2} = \frac{y_2'}{y_1} - \frac{y_1'}{y_1^2}y_2 = \frac{y_2'}{y_1} + \left[\frac{d}{dz}\left(\frac{1}{y_1}\right)\right]y_2 = \frac{d}{dz}\left(\frac{y_2}{y_1}\right),$$

which integrates to give

$$y_2(z) = y_1(z)\int^z \frac{W(u)}{y_1^2(u)}\,du.$$

Now using the alternative expression for $W(z)$ given in (16.4) with $C = 1$ (since we are not concerned with this normalising factor), we find

$$y_2(z) = y_1(z)\int^z \frac{1}{y_1^2(u)}\exp\left\{-\int^u p(v)\,dv\right\}du. \tag{16.25}$$

Hence, given y_1, we can in principle compute y_2. Note that the lower limits of integration have been omitted. If constant lower limits are included then they merely lead to a constant times the first solution.

►*Find a second solution to (16.21) using the Wronskian method.*

For the ODE (16.21) we have $p(z) = 3/(z-1)$, and from (16.24) we see that one solution to (16.21) is $y_1 = z/(1-z)^2$. Substituting for p and y_1 in (16.25) we have

$$\begin{aligned}
y_2(z) &= \frac{z}{(1-z)^2} \int^z \frac{(1-u)^4}{u^2} \exp\left(-\int^u \frac{3}{v-1}\,dv\right) du \\
&= \frac{z}{(1-z)^2} \int^z \frac{(1-u)^4}{u^2} \exp\left[-3\ln(u-1)\right] du \\
&= \frac{z}{(1-z)^2} \int^z \frac{u-1}{u^2}\, du \\
&= \frac{z}{(1-z)^2} \left(\ln z + \frac{1}{z}\right).
\end{aligned}$$

By calculating the Wronskian of y_1 and y_2 it is easily shown that, as expected, the two solutions are linearly independent. In fact, as the Wronskian has already been evaluated as $W(u) = \exp[-3\ln(u-1)]$, i.e. $W(z) = (z-1)^{-3}$, no calculation is needed. ◄

An alternative (but equivalent) method of finding a second solution is simply to assume that the second solution has the form $y_2(z) = u(z)y_1(z)$ for some function $u(z)$ to be determined (this method was discussed more fully in subsection 15.2.3). From (16.25), we see that the second solution derived from the Wronskian is indeed of this form. Substituting $y_2(z) = u(z)y_1(z)$ into the ODE leads to a first-order ODE in which u' is the dependent variable; this may then be solved.

16.4.2 The derivative method

The derivative method of finding a second solution begins with the derivation of a recurrence relation for the coefficients a_n in a Frobenius series solution, as in the previous section. However, rather than putting $\sigma = \sigma_1$ in this recurrence relation to evaluate the first series solution, we now keep σ as a variable parameter. This means that the computed a_n are functions of σ and the computed solution is now a function of z and σ:

$$y(z,\sigma) = z^\sigma \sum_{n=0}^{\infty} a_n(\sigma) z^n. \tag{16.26}$$

Of course, if we put $\sigma = \sigma_1$ in this, we obtain immediately the first series solution, but for the moment we leave σ as a parameter.

For brevity let us denote the differential operator on the LHS of our standard ODE (16.7) by $\mathcal{L}$, so that

$$\mathcal{L} = \frac{d^2}{dz^2} + p(z)\frac{d}{dz} + q(z),$$

and examine the effect of $\mathcal{L}$ on the series $y(z,\sigma)$ in (16.26). It is clear that the series $\mathcal{L}y(z,\sigma)$ will contain only a term in z^σ, since the recurrence relation defining the $a_n(\sigma)$ is such that these coefficients vanish for higher powers of z. But the coefficient of z^σ is simply the LHS of the indicial equation. Therefore, if the roots of the indicial equation are $\sigma = \sigma_1$ and $\sigma = \sigma_2$ then it follows that

$$\mathcal{L}y(z,\sigma) = a_0(\sigma - \sigma_1)(\sigma - \sigma_2)z^\sigma. \tag{16.27}$$

Therefore, as in the previous section, we see that for $y(z,\sigma)$ to be a solution of the ODE $\mathcal{L}y = 0$, σ must equal σ_1 or σ_2. For simplicity we shall set $a_0 = 1$ in the following discussion.

Let us first consider the case in which the two roots of the indicial equation are equal, i.e. $\sigma_2 = \sigma_1$. From (16.27) we then have

$$\mathcal{L}y(z,\sigma) = (\sigma - \sigma_1)^2 z^\sigma.$$

Differentiating this equation with respect to σ we obtain

$$\frac{\partial}{\partial\sigma}\left[\mathcal{L}y(z,\sigma)\right] = (\sigma - \sigma_1)^2 z^\sigma \ln z + 2(\sigma - \sigma_1)z^\sigma,$$

which equals zero if $\sigma = \sigma_1$. But since $\partial/\partial\sigma$ and $\mathcal{L}$ are operators that differentiate with respect to different variables, we can reverse their order, implying that

$$\mathcal{L}\left[\frac{\partial}{\partial\sigma}y(z,\sigma)\right] = 0 \qquad \text{at } \sigma = \sigma_1.$$

Hence, the function in square brackets, evaluated at $\sigma = \sigma_1$ and denoted by

$$\left[\frac{\partial}{\partial\sigma}y(z,\sigma)\right]_{\sigma=\sigma_1}, \tag{16.28}$$

is also a solution of the original ODE $\mathcal{L}y = 0$, and is in fact the second linearly independent solution that we were looking for.

The case in which the roots of the indicial equation differ by an integer is slightly more complicated but can be treated in a similar way. In (16.27), since $\mathcal{L}$ differentiates with respect to z we may multiply (16.27) by any function of σ, say $\sigma - \sigma_2$, and take this function inside the operator $\mathcal{L}$ on the LHS to obtain

$$\mathcal{L}\left[(\sigma - \sigma_2)y(z,\sigma)\right] = (\sigma - \sigma_1)(\sigma - \sigma_2)^2 z^\sigma. \tag{16.29}$$

Therefore the function

$$\left[(\sigma - \sigma_2)y(z,\sigma)\right]_{\sigma=\sigma_2}$$

is also a solution of the ODE $\mathcal{L}y = 0$. However, it can be proved[§] that this function is a simple multiple of the first solution $y(z,\sigma_1)$, showing that it is not linearly independent and that we must find another solution. To do this we differentiate (16.29) with respect to σ and find

$$\begin{aligned}\frac{\partial}{\partial\sigma}\left\{\mathcal{L}\left[(\sigma - \sigma_2)y(z,\sigma)\right]\right\} &= (\sigma - \sigma_2)^2 z^\sigma + 2(\sigma - \sigma_1)(\sigma - \sigma_2)z^\sigma \\ &\quad + (\sigma - \sigma_1)(\sigma - \sigma_2)^2 z^\sigma \ln z,\end{aligned}$$

[§] For a fuller discussion see, for example, K. F. Riley, *Mathematical Methods for the Physical Sciences* (Cambridge: Cambridge University Press, 1974), pp. 158–9.

which is equal to zero if $\sigma = \sigma_2$. As previously, since $\partial/\partial\sigma$ and $\mathcal{L}$ are operators that differentiate with respect to different variables, we can reverse their order to obtain

$$\mathcal{L}\left\{\frac{\partial}{\partial\sigma}\left[(\sigma-\sigma_2)y(z,\sigma)\right]\right\} = 0 \qquad \text{at } \sigma = \sigma_2,$$

and so the function

$$\left\{\frac{\partial}{\partial\sigma}\left[(\sigma-\sigma_2)y(z,\sigma)\right]\right\}_{\sigma=\sigma_2} \tag{16.30}$$

is also a solution of the original ODE $\mathcal{L}y = 0$, and is in fact the second linearly independent solution.

►*Find a second solution to (16.21) using the derivative method.*

From (16.23) the recurrence relation (with σ as a parameter) is given by

$$(n+\sigma-1)a_n = (n+\sigma)a_{n-1}.$$

Setting $a_0 = 1$ we find that the coefficients have the particularly simple form $a_n(\sigma) = (\sigma+n)/\sigma$. We therefore consider the function

$$y(z,\sigma) = z^\sigma \sum_{n=0}^{\infty} a_n(\sigma)z^n = z^\sigma \sum_{n=0}^{\infty} \frac{\sigma+n}{\sigma} z^n.$$

The smaller root of the indicial equation for (16.21) is $\sigma_2 = 0$, and so from (16.30) a second, linearly independent, solution to the ODE is given by

$$\left\{\frac{\partial}{\partial\sigma}\left[\sigma y(z,\sigma)\right]\right\}_{\sigma=0} = \left\{\frac{\partial}{\partial\sigma}\left[z^\sigma \sum_{n=0}^{\infty}(\sigma+n)z^n\right]\right\}_{\sigma=0}.$$

The derivative with respect to σ is given by

$$\frac{\partial}{\partial\sigma}\left[z^\sigma \sum_{n=0}^{\infty}(\sigma+n)z^n\right] = z^\sigma \ln z \sum_{n=0}^{\infty}(\sigma+n)z^n + z^\sigma \sum_{n=0}^{\infty} z^n,$$

which on setting $\sigma = 0$ gives the second solution

$$\begin{aligned} y_2(z) &= \ln z \sum_{n=0}^{\infty} nz^n + \sum_{n=0}^{\infty} z^n \\ &= \frac{z}{(1-z)^2}\ln z + \frac{1}{1-z} \\ &= \frac{z}{(1-z)^2}\left(\ln z + \frac{1}{z} - 1\right). \end{aligned}$$

This second solution is the same as that obtained by the Wronskian method in the previous subsection except for the addition of some of the first solution. ◄

16.4.3 Series form of the second solution

Using any of the methods discussed above, we can find the general form of the second solution to the ODE. This form is most easily found, however, using the derivative method. Let us first consider the case where the two solutions of the indicial equation are equal. In this case a second solution is given by (16.28), which may be written as

$$\begin{aligned}
y_2(z) &= \left[\frac{\partial y(z,\sigma)}{\partial \sigma}\right]_{\sigma=\sigma_1} \\
&= (\ln z) z^{\sigma_1} \sum_{n=0}^{\infty} a_n(\sigma_1) z^n + z^{\sigma_1} \sum_{n=1}^{\infty} \left[\frac{da_n(\sigma)}{d\sigma}\right]_{\sigma=\sigma_1} z^n \\
&= y_1(z) \ln z + z^{\sigma_1} \sum_{n=1}^{\infty} b_n z^n, \qquad (16.31)
\end{aligned}$$

where $b_n = [da_n(\sigma)/d\sigma]_{\sigma=\sigma_1}$. One could equally obtain the coefficients b_n by direct substitution of the form (16.31) into the original ODE.

In the case where the roots of the indicial equation differ by an integer (not equal to zero), then from (16.30) a second solution is given by

$$\begin{aligned}
y_2(z) &= \left\{\frac{\partial}{\partial \sigma}\left[(\sigma - \sigma_2) y(z,\sigma)\right]\right\}_{\sigma=\sigma_2} \\
&= \ln z \left[(\sigma - \sigma_2) z^{\sigma} \sum_{n=0}^{\infty} a_n(\sigma) z^n\right]_{\sigma=\sigma_2} + z^{\sigma_2} \sum_{n=0}^{\infty} \left[\frac{d}{d\sigma}(\sigma - \sigma_2) a_n(\sigma)\right]_{\sigma=\sigma_2} z^n.
\end{aligned}$$

But, as we mentioned in the previous section, $[(\sigma - \sigma_2) y(z,\sigma)]$ at $\sigma = \sigma_2$ is just a multiple of the first solution $y(z, \sigma_1)$. Therefore the second solution is of the form

$$y_2(z) = c y_1(z) \ln z + z^{\sigma_2} \sum_{n=0}^{\infty} b_n z^n, \qquad (16.32)$$

where c is a constant. In some cases, however, c might be zero, and so the second solution would not contain the term in $\ln z$ and could be written simply as a Frobenius series. Clearly this corresponds to the case in which the substitution of a Frobenius series into the original ODE yields two solutions automatically. In either case, the coefficients b_n may also be found by direct substitution of the form (16.32) into the original ODE.

16.5 Polynomial solutions

We have seen that the evaluation of successive terms of a series solution to a differential equation is carried out by means of a recurrence relation. The form of the relation for a_n depends upon n, the previous values of a_r ($r < n$) and the parameters of the equation. It may happen, as a result of this, that for some value of $n = N + 1$ the computed value a_{N+1} is zero and that all higher a_r also vanish. If this is so, and the corresponding solution of the indicial equation σ

is a positive integer or zero, then we are left with a finite polynomial of degree $N' = N + \sigma$ as a solution of the ODE:

$$y(z) = \sum_{n=0}^{N} a_n z^{n+\sigma}. \tag{16.33}$$

In many applications in theoretical physics (particularly in quantum mechanics) the termination of a potentially infinite series after a finite number of terms is of crucial importance in establishing physically acceptable descriptions and properties of systems. The condition under which such a termination occurs is therefore of considerable importance.

►*Find power series solutions about $z = 0$ of*

$$y'' - 2zy' + \lambda y = 0. \tag{16.34}$$

For what values of λ does the equation possess a polynomial solution? Find such a solution for $\lambda = 4$.

Clearly $z = 0$ is an ordinary point of (16.34) and so we look for solutions of the form $y = \sum_{n=0}^{\infty} a_n z^n$. Substituting this into the ODE and multiplying through by z^2 we find

$$\sum_{n=0}^{\infty} [n(n-1) - 2z^2 n + \lambda z^2] a_n z^n = 0.$$

By demanding that the coefficients of each power of z vanish separately we derive the recurrence relation

$$n(n-1)a_n - 2(n-2)a_{n-2} + \lambda a_{n-2} = 0,$$

which may be rearranged to give

$$a_n = \frac{2(n-2) - \lambda}{n(n-1)} a_{n-2} \qquad \text{for } n \geq 2. \tag{16.35}$$

The odd and even coefficients are therefore independent of one another, and two solutions to (16.34) may be derived. We either set $a_1 = 0$ and $a_0 = 1$ to obtain

$$y_1(z) = 1 - \lambda \frac{z^2}{2!} - \lambda(4-\lambda)\frac{z^4}{4!} - \lambda(4-\lambda)(8-\lambda)\frac{z^6}{6!} - \cdots \tag{16.36}$$

or set $a_0 = 0$ and $a_1 = 1$ to obtain

$$y_2(z) = z + (2-\lambda)\frac{z^3}{3!} + (2-\lambda)(6-\lambda)\frac{z^5}{5!} + (2-\lambda)(6-\lambda)(10-\lambda)\frac{z^7}{7!} + \cdots.$$

Now, from the recurrence relation (16.35) (or in this case from the expressions for y_1 and y_2 themselves) we see that for the ODE to possess a polynomial solution we require $\lambda = 2(n-2)$ for $n \geq 2$ or, more simply, $\lambda = 2n$ for $n \geq 0$, i.e. λ must be an even positive integer. If $\lambda = 4$ then from (16.36) the ODE has the polynomial solution

$$y_1(z) = 1 - \frac{4z^2}{2!} = 1 - 2z^2. \blacktriangleleft$$

A simpler method of obtaining finite polynomial solutions is to *assume* a solution of the form (16.33), where $a_N \neq 0$. Instead of starting with the lowest power of z, as we have done up to now, this time we start by considering the coefficient of the highest power z^N; such a power now exists because of our assumed form of solution.

►*By assuming a polynomial solution find the values of λ in (16.34) for which such a solution exists.*

We assume a polynomial solution to (16.34) of the form $y = \sum_{n=0}^{N} a_n z^n$. Substituting this form into (16.34) we find

$$\sum_{n=0}^{N} \left[n(n-1)a_n z^{n-2} - 2zna_n z^{n-1} + \lambda a_n z^n \right] = 0.$$

Now, instead of starting with the lowest power of z, we start with the highest. Thus, demanding that the coefficient of z^N vanishes, we require $-2N + \lambda = 0$, i.e. $\lambda = 2N$, as we found in the previous example. By demanding that the coefficient of a general power of z is zero, the same recurrence relation as above may be derived and the solutions found. ◄

16.6 Exercises

16.1 Find two power series solutions about $z = 0$ of the differential equation

$$(1 - z^2)y'' - 3zy' + \lambda y = 0.$$

Deduce that the value of λ for which the corresponding power series becomes an Nth-degree polynomial $U_N(z)$ is $N(N + 2)$. Construct $U_2(z)$ and $U_3(z)$.

16.2 Find solutions, as power series in z, of the equation

$$4zy'' + 2(1 - z)y' - y = 0.$$

Identify one of the solutions and verify it by direct substitution.

16.3 Find power series solutions in z of the differential equation

$$zy'' - 2y' + 9z^5 y = 0.$$

Identify closed forms for the two series, calculate their Wronskian, and verify that they are linearly independent. Compare the Wronskian with that calculated from the differential equation.

16.4 Change the independent variable in the equation

$$\frac{d^2f}{dz^2} + 2(z - a)\frac{df}{dz} + 4f = 0 \qquad (*)$$

from z to $x = z - \alpha$, and find two independent series solutions, expanded about $x = 0$, of the resulting equation. Deduce that the general solution of $(*)$ is

$$f(z, \alpha) = A(z - \alpha)e^{-(z-\alpha)^2} + B\sum_{m=0}^{\infty} \frac{(-4)^m m!}{(2m)!}(z - \alpha)^{2m},$$

with A and B arbitrary constants.

16.5 Investigate solutions of Legendre's equation at one of its singular points as follows.

(a) Verify that $z = 1$ is a regular singular point of Legendre's equation and that the indicial equation for a series solution in powers of $(z - 1)$ has roots 0 and 3.

(b) Obtain the corresponding recurrence relation and show that $\sigma = 0$ does not give a valid series solution.

(c) Determine the radius of convergence R of the $\sigma = 3$ series and relate it to the positions of the singularities of Legendre's equation.

16.6 Verify that $z = 0$ is a regular singular point of the equation

$$z^2 y'' - \tfrac{3}{2} z y' + (1 + z)y = 0,$$

and that the indicial equation has roots 2 and 1/2. Show that the general solution is given by

$$y(z) = 6a_0 z^2 \sum_{n=0}^{\infty} \frac{(-1)^n (n+1) 2^{2n} z^n}{(2n+3)!}$$
$$+ b_0 \left(z^{1/2} + 2z^{3/2} - \frac{z^{1/2}}{4} \sum_{n=2}^{\infty} \frac{(-1)^n 2^{2n} z^n}{n(n-1)(2n-3)!} \right).$$

16.7 Use the derivative method to obtain, as a second solution of Bessel's equation for the case when $\nu = 0$, the following expression:

$$J_0(z) \ln z - \sum_{n=1}^{\infty} \frac{(-1)^n}{(n!)^2} \left(\sum_{r=1}^{n} \frac{1}{r} \right) \left(\frac{z}{2} \right)^{2n},$$

given that the first solution is $J_0(z)$, as specified by (18.79).

16.8 Consider a series solution of the equation

$$zy'' - 2y' + yz = 0 \qquad (*)$$

about its regular singular point.

(a) Show that its indicial equation has roots that differ by an integer but that the two roots nevertheless generate linearly independent solutions

$$y_1(z) = 3a_0 \sum_{n=1}^{\infty} \frac{(-1)^{n+1}\, 2nz^{2n+1}}{(2n+1)!},$$

$$y_2(z) = a_0 \sum_{n=0}^{\infty} \frac{(-1)^{n+1}(2n-1)z^{2n}}{(2n)!}.$$

(b) Show that $y_1(z)$ is equal to $3a_0(\sin z - z\cos z)$ by expanding the sinusoidal functions. Then, using the Wronskian method, find an expression for $y_2(z)$ in terms of sinusoids. You will need to write z^2 as $(z/\sin z)(z \sin z)$ and integrate by parts to evaluate the integral involved.

(c) Confirm that the two solutions are linearly independent by showing that their Wronskian is equal to $-z^2$, as would be expected from the form of $(*)$.

16.9 Find series solutions of the equation $y'' - 2zy' - 2y = 0$. Identify one of the series as $y_1(z) = \exp z^2$ and verify this by direct substitution. By setting $y_2(z) = u(z)y_1(z)$ and solving the resulting equation for $u(z)$, find an explicit form for $y_2(z)$ and deduce that

$$\int_0^x e^{-v^2}\, dv = e^{-x^2} \sum_{n=0}^{\infty} \frac{n!}{2(2n+1)!}(2x)^{2n+1}.$$

16.10 Solve the equation

$$z(1-z)\frac{d^2y}{dz^2} + (1-z)\frac{dy}{dz} + \lambda y = 0$$

as follows.

(a) Identify and classify its singular points and determine their indices.

(b) Find one series solution in powers of z. Give a formal expression for a second linearly independent solution.

(c) Deduce the values of λ for which there is a polynomial solution $P_N(z)$ of degree N. Evaluate the first four polynomials, normalised in such a way that $P_N(0) = 1$.

16.11 Find the general power series solution about $z = 0$ of the equation

$$z\frac{d^2y}{dz^2} + (2z-3)\frac{dy}{dz} + \frac{4}{z}y = 0.$$

16.12 Find the radius of convergence of a series solution about the origin for the equation $(z^2 + az + b)y'' + 2y = 0$ in the following cases:

$$\text{(a) } a = 5,\ b = 6; \qquad \text{(b) } a = 5,\ b = 7.$$

Show that if a and b are real and $4b > a^2$, then the radius of convergence is always given by $b^{1/2}$.

16.13 For the equation $y'' + z^{-3}y = 0$, show that the origin becomes a regular singular point if the independent variable is changed from z to $x = 1/z$. Hence find a series solution of the form $y_1(z) = \sum_0^\infty a_n z^{-n}$. By setting $y_2(z) = u(z)y_1(z)$ and expanding the resulting expression for du/dz in powers of z^{-1}, show that $y_2(z)$ has the asymptotic form

$$y_2(z) = c\left[z + \ln z - \tfrac{1}{2} + O\left(\frac{\ln z}{z}\right)\right],$$

where c is an arbitrary constant.

16.14 Prove that the Laguerre equation,

$$z\frac{d^2y}{dz^2} + (1-z)\frac{dy}{dz} + \lambda y = 0,$$

has polynomial solutions $L_N(z)$ if λ is a non-negative integer N, and determine the recurrence relationship for the polynomial coefficients. Hence show that an expression for $L_N(z)$, normalised in such a way that $L_N(0) = N!$, is

$$L_N(z) = \sum_{n=0}^{N} \frac{(-1)^n (N!)^2}{(N-n)!(n!)^2} z^n.$$

Evaluate $L_3(z)$ explicitly.

16.15 The origin is an ordinary point of the Chebyshev equation,

$$(1-z^2)y'' - zy' + m^2 y = 0,$$

which therefore has series solutions of the form $z^\sigma \sum_0^\infty a_n z^n$ for $\sigma = 0$ and $\sigma = 1$.

(a) Find the recurrence relationships for the a_n in the two cases and show that there exist polynomial solutions $T_m(z)$:

(i) for $\sigma = 0$, when m is an even integer, the polynomial having $\frac{1}{2}(m+2)$ terms;

(ii) for $\sigma = 1$, when m is an odd integer, the polynomial having $\frac{1}{2}(m+1)$ terms.

(b) $T_m(z)$ is normalised so as to have $T_m(1) = 1$. Find explicit forms for $T_m(z)$ for $m = 0, 1, 2, 3$.

(c) Show that the corresponding non-terminating series solutions $S_m(z)$ have as their first few terms

$$S_0(z) = a_0\left(z + \frac{1}{3!}z^3 + \frac{9}{5!}z^5 + \cdots\right),$$
$$S_1(z) = a_0\left(1 - \frac{1}{2!}z^2 - \frac{3}{4!}z^4 - \cdots\right),$$
$$S_2(z) = a_0\left(z - \frac{3}{3!}z^3 - \frac{15}{5!}z^5 - \cdots\right),$$
$$S_3(z) = a_0\left(1 - \frac{9}{2!}z^2 + \frac{45}{4!}z^4 + \cdots\right).$$

16.16 Obtain the recurrence relations for the solution of Legendre's equation (18.1) in *inverse* powers of z, i.e. set $y(z) = \sum a_n z^{\sigma-n}$, with $a_0 \neq 0$. Deduce that, if ℓ is an integer, then the series with $\sigma = \ell$ will terminate and hence converge for all z, whilst the series with $\sigma = -(\ell + 1)$ does not terminate and hence converges only for $|z| > 1$.

16.7 Hints and answers

16.1 Note that $z = 0$ is an ordinary point of the equation.
For $\sigma = 0$, $a_{n+2}/a_n = [n(n+2) - \lambda]/[(n+1)(n+2)]$ and, correspondingly, for $\sigma = 1$, $U_2(z) = a_0(1 - 4z^2)$ and $U_3(z) = a_0(z - 2z^3)$.

16.3 $\sigma = 0$ and 3; $a_{6m}/a_0 = (-1)^m/(2m)!$ and $a_{6m}/a_0 = (-1)^m/(2m+1)!$, respectively. $y_1(z) = a_0 \cos z^3$ and $y_2(z) = a_0 \sin z^3$. The Wronskian is $\pm 3a_0^2 z^2 \neq 0$.

16.5 (b) $a_{n+1}/a_n = [\ell(\ell+1) - n(n+1)]/[2(n+1)^2]$.
(c) $R = 2$, equal to the distance between $z = 1$ and the closest singularity at $z = -1$.

16.7 A typical term in the series for $y(\sigma, z)$ is $\dfrac{(-1)^n z^{2n}}{[(\sigma+2)(\sigma+4)\cdots(\sigma+2n)]^2}$.

16.9 The origin is an ordinary point. Determine the constant of integration by examining the behaviour of the related functions for small x.
$y_2(z) = (\exp z^2)\int_0^z \exp(-x^2)\,dx$.

16.11 Repeated roots $\sigma = 2$.

$$y(z) = az^2 - 4az^3 + 6bz^3 + \sum_{n=2}^{\infty} \frac{(n+1)(-2z)^{n+2}}{n!}\left\{\frac{a}{4} + b\,[\ln z + g(n)]\right\},$$

where

$$g(n) = \frac{1}{n+1} - \frac{1}{n} - \frac{1}{n-1} - \cdots - \frac{1}{2} - 2.$$

16.13 The transformed equation is $xy'' + 2y' + y = 0$; $a_n = (-1)^n(n+1)^{-1}(n!)^{-2}a_0$; $du/dz = A[y_1(z)]^{-2}$.

16.15 (a) (i) $a_{n+2} = [a_n(n^2 - m^2)]/[(n+2)(n+1)]$,
(ii) $a_{n+2} = \{a_n[(n+1)^2 - m^2]\}/[(n+3)(n+2)]$; (b) 1, z, $2z^2 - 1$, $4z^3 - 3z$.

17

Eigenfunction methods for differential equations

In the previous three chapters we dealt with the solution of differential equations of order n by two methods. In one method, we found n independent solutions of the equation and then combined them, weighted with coefficients determined by the boundary conditions; in the other we found solutions in terms of series whose coefficients were related by (in general) an n-term recurrence relation and thence fixed by the boundary conditions. For both approaches the linearity of the equation was an important or essential factor in the utility of the method, and in this chapter our aim will be to exploit the superposition properties of linear differential equations even further.

We will be concerned with the solution of equations of the inhomogeneous form

$$\mathcal{L}y(x) = f(x), \tag{17.1}$$

where $f(x)$ is a prescribed or general function *and* the boundary conditions to be satisfied by the solution $y = y(x)$, for example at the limits $x = a$ and $x = b$, are given. The expression $\mathcal{L}y(x)$ stands for a linear differential operator $\mathcal{L}$ acting upon the function $y(x)$.

In general, unless $f(x)$ is both known and simple, it will not be possible to find particular integrals of (17.1), even if complementary functions can be found that satisfy $\mathcal{L}y = 0$. The idea is therefore to exploit the linearity of $\mathcal{L}$ by building up the required solution $y(x)$ as a *superposition*, generally containing an infinite number of terms, of some set of functions $\{y_i(x)\}$ that each individually satisfy the boundary conditions. Clearly this brings in a quite considerable complication but since, within reason, we may select the set of functions to suit ourselves, we can obtain sizeable compensation for this complication. Indeed, if the set chosen is one containing functions that, when acted upon by $\mathcal{L}$, produce particularly simple results then we can 'show a profit' on the operation. In particular, if the set consists of those functions y_i for which

$$\mathcal{L}y_i(x) = \lambda_i y_i(x), \tag{17.2}$$

where λ_i is a constant (and which satisfy the boundary conditions), then a distinct advantage may be obtained from the manoeuvre because all the differentiation will have disappeared from (17.1).

Equation (17.2) is clearly reminiscent of the equation satisfied by the *eigenvectors* $\mathbf{x}^i$ of a linear operator $\mathcal{A}$, namely

$$\mathcal{A}\mathbf{x}^i = \lambda_i \mathbf{x}^i, \tag{17.3}$$

where λ_i is a constant and is called the *eigenvalue* associated with $\mathbf{x}^i$. By analogy, in the context of differential equations a function $y_i(x)$ satisfying (17.2) is called an *eigenfunction* of the operator $\mathcal{L}$ (under the imposed boundary conditions) and λ_i is then called the eigenvalue associated with the eigenfunction $y_i(x)$. Clearly, the eigenfunctions $y_i(x)$ of $\mathcal{L}$ are only determined up to an arbitrary scale factor by (17.2).

Probably the most familiar equation of the form (17.2) is that which describes a simple harmonic oscillator, i.e.

$$\mathcal{L}y \equiv -\frac{d^2y}{dt^2} = \omega^2 y, \qquad \text{where } \mathcal{L} \equiv -d^2/dt^2. \tag{17.4}$$

Imposing the boundary condition that the solution is periodic with period T, the eigenfunctions in this case are given by $y_n(t) = A_n e^{i\omega_n t}$, where $\omega_n = 2\pi n/T$, $n = 0, \pm1, \pm2, \ldots$ and the A_n are constants. The eigenvalues are $\omega_n^2 = n^2\omega_1^2 = n^2(2\pi/T)^2$. (Sometimes ω_n is referred to as the eigenvalue of this equation, but we will avoid such confusing terminology here.)

We may discuss a somewhat wider class of differential equations by considering a slightly more general form of (17.2), namely

$$\mathcal{L}y_i(x) = \lambda_i \rho(x) y_i(x), \tag{17.5}$$

where $\rho(x)$ is a *weight function*. In many applications $\rho(x)$ is unity for all x, in which case (17.2) is recovered; in general, though, it is a function determined by the choice of coordinate system used in describing a particular physical situation. The only requirement on $\rho(x)$ is that it is real and does not change sign in the range $a \leq x \leq b$, so that it can, without loss of generality, be taken to be non-negative throughout; of course, $\rho(x)$ must be the same function for all values of λ_i. A function $y_i(x)$ that satisfies (17.5) is called an eigenfunction of the operator $\mathcal{L}$ with respect to the weight function $\rho(x)$.

This chapter will not cover methods used to determine the eigenfunctions of (17.2) or (17.5), since we have discussed those in previous chapters, but, rather, will use the properties of the eigenfunctions to solve inhomogeneous equations of the form (17.1). We shall see later that the sets of eigenfunctions $y_i(x)$ of a particular class of operators called *Hermitian operators* (the operator in the simple harmonic oscillator equation is an example) have particularly useful properties and these will be studied in detail. It turns out that many of the interesting differential operators met within the physical sciences are Hermitian. Before continuing our discussion of the eigenfunctions of Hermitian operators, however, we will consider some properties of general sets of functions.

17.1 Sets of functions

In chapter 8 we discussed the definition of a vector space but concentrated on spaces of finite dimensionality. We consider now the *infinite*-dimensional space of all reasonably well-behaved functions $f(x)$, $g(x)$, $h(x)$, ... on the interval $a \leq x \leq b$. That these functions form a linear vector space is shown by noting the following properties. The set is closed under

(i) addition, which is commutative and associative, i.e.

$$f(x) + g(x) = g(x) + f(x),$$
$$[f(x) + g(x)] + h(x) = f(x) + [g(x) + h(x)],$$

(ii) multiplication by a scalar, which is distributive and associative, i.e.

$$\lambda [f(x) + g(x)] = \lambda f(x) + \lambda g(x),$$
$$\lambda [\mu f(x)] = (\lambda \mu) f(x),$$
$$(\lambda + \mu) f(x) = \lambda f(x) + \mu f(x).$$

Furthermore, in such a space

(iii) there exists a 'null vector' 0 such that $f(x) + 0 = f(x)$,
(iv) multiplication by unity leaves any function unchanged, i.e. $1 \times f(x) = f(x)$,
(v) each function has an associated negative function $-f(x)$ that is such that $f(x) + [-f(x)] = 0$.

By analogy with finite-dimensional vector spaces we now introduce a set of linearly independent basis functions $y_n(x)$, $n = 0, 1, \ldots, \infty$, such that *any* 'reasonable' function in the interval $a \leq x \leq b$ (i.e. it obeys the Dirichlet conditions discussed in chapter 12) can be expressed as the linear sum of these functions:

$$f(x) = \sum_{n=0}^{\infty} c_n y_n(x).$$

Clearly if a different set of linearly independent basis functions $u_n(x)$ is chosen then the function can be expressed in terms of the new basis,

$$f(x) = \sum_{n=0}^{\infty} d_n u_n(x),$$

where the d_n are a different set of coefficients. In each case, provided the basis functions are linearly independent, the coefficients are unique.

We may also define an *inner product* on our function space by

$$\langle f|g\rangle = \int_a^b f^*(x)g(x)\rho(x)\,dx, \tag{17.6}$$

where $\rho(x)$ is the weight function, which we require to be real and non-negative in the interval $a \le x \le b$. As mentioned above, $\rho(x)$ is often unity for all x. Two functions are said to be *orthogonal* (with respect to the weight function $\rho(x)$) on the interval $[a, b]$ if

$$\langle f|g\rangle = \int_a^b f^*(x)g(x)\rho(x)\,dx = 0, \tag{17.7}$$

and the *norm* of a function is defined as

$$\|f\| = \langle f|f\rangle^{1/2} = \left[\int_a^b f^*(x)f(x)\rho(x)\,dx\right]^{1/2} = \left[\int_a^b |f(x)|^2\rho(x)\,dx\right]^{1/2}. \tag{17.8}$$

It is also common practice to define a *normalised* function by $\hat{f} = f/\|f\|$, which has unit norm.

An infinite-dimensional vector space of functions, for which an inner product is defined, is called a *Hilbert space*. Using the concept of the inner product, we can choose a basis of linearly independent functions $\hat{\phi}_n(x)$, $n = 0, 1, 2, \ldots$ that are orthonormal, i.e. such that

$$\langle \hat{\phi}_i|\hat{\phi}_j\rangle = \int_a^b \hat{\phi}_i^*(x)\hat{\phi}_j(x)\rho(x)\,dx = \delta_{ij}. \tag{17.9}$$

If $y_n(x)$, $n = 0, 1, 2, \ldots$, are a linearly independent, but not orthonormal, basis for the Hilbert space then an orthonormal set of basis functions $\hat{\phi}_n$ may be produced (in a similar manner to that used in the construction of a set of orthogonal eigenvectors of an Hermitian matrix; see chapter 8) by the following procedure:

$$\begin{aligned}
\phi_0 &= y_0,\\
\phi_1 &= y_1 - \hat{\phi}_0\langle\hat{\phi}_0|y_1\rangle,\\
\phi_2 &= y_2 - \hat{\phi}_1\langle\hat{\phi}_1|y_2\rangle - \hat{\phi}_0\langle\hat{\phi}_0|y_2\rangle,\\
&\ \vdots\\
\phi_n &= y_n - \hat{\phi}_{n-1}\langle\hat{\phi}_{n-1}|y_n\rangle - \cdots - \hat{\phi}_0\langle\hat{\phi}_0|y_n\rangle,\\
&\ \vdots
\end{aligned}$$

It is straightforward to check that each ϕ_n is orthogonal to all its predecessors ϕ_i, $i = 0, 1, 2, \ldots, n-1$. This method is called *Gram–Schmidt orthogonalisation.* Clearly the functions ϕ_n form an orthogonal set, but in general they do not have unit norms.

►*Starting from the linearly independent functions $y_n(x) = x^n$, $n = 0, 1, \ldots$, construct three orthonormal functions over the range $-1 < x < 1$, assuming a weight function of unity.*

The first unnormalised function ϕ_0 is simply equal to the first of the original functions, i.e.

$$\phi_0 = 1.$$

The normalisation is carried out by dividing by

$$\langle \phi_0 | \phi_0 \rangle^{1/2} = \left(\int_{-1}^{1} 1 \times 1 \, du \right)^{1/2} = \sqrt{2},$$

with the result that the first normalised function $\hat{\phi}_0$ is given by

$$\hat{\phi}_0 = \frac{\phi_0}{\sqrt{2}} = \sqrt{\tfrac{1}{2}}.$$

The second unnormalised function is found by applying the above Gram–Schmidt orthogonalisation procedure, i.e.

$$\phi_1 = y_1 - \hat{\phi}_0 \langle \hat{\phi}_0 | y_1 \rangle.$$

It can easily be shown that $\langle \hat{\phi}_0 | y_1 \rangle = 0$, and so $\phi_1 = x$. Normalising then gives

$$\hat{\phi}_1 = \phi_1 \left(\int_{-1}^{1} u \times u \, du \right)^{-1/2} = \sqrt{\tfrac{3}{2}} x.$$

The third unnormalised function is similarly given by

$$\begin{aligned} \phi_2 &= y_2 - \hat{\phi}_1 \langle \hat{\phi}_1 | y_2 \rangle - \hat{\phi}_0 \langle \hat{\phi}_0 | y_2 \rangle \\ &= x^2 - 0 - \tfrac{1}{3}, \end{aligned}$$

which, on normalising, gives

$$\hat{\phi}_2 = \phi_2 \left(\int_{-1}^{1} \left(u^2 - \tfrac{1}{3} \right)^2 du \right)^{-1/2} = \tfrac{1}{2} \sqrt{\tfrac{5}{2}} (3x^2 - 1).$$

By comparing the functions $\hat{\phi}_0$, $\hat{\phi}_1$ and $\hat{\phi}_2$ with the list in subsection 18.1.1, we see that this procedure has generated (multiples of) the first three Legendre polynomials. ◄

If a function is expressed in terms of an *orthonormal* basis $\hat{\phi}_n(x)$ as

$$f(x) = \sum_{n=0}^{\infty} c_n \hat{\phi}_n(x) \tag{17.10}$$

then the coefficients c_n are given by

$$c_n = \langle \hat{\phi}_n | f \rangle = \int_a^b \hat{\phi}_n^*(x) f(x) \rho(x) \, dx. \tag{17.11}$$

Note that this is true only if the basis is orthonormal.

17.1.1 Some useful inequalities

Since for a Hilbert space $\langle f|f\rangle \geq 0$, the inequalities discussed in subsection 8.1.3 hold. The proofs are not repeated here, but the relationships are listed for completeness.

(i) The Schwarz inequality states that

$$|\langle f|g\rangle| \leq \langle f|f\rangle^{1/2}\langle g|g\rangle^{1/2}, \tag{17.12}$$

where the equality holds when $f(x)$ is a scalar multiple of $g(x)$, i.e. when they are linearly dependent.

(ii) The triangle inequality states that

$$\|f+g\| \leq \|f\| + \|g\|, \tag{17.13}$$

where again equality holds when $f(x)$ is a scalar multiple of $g(x)$.

(iii) Bessel's inequality requires the introduction of an *orthonormal* basis $\hat{\phi}_n(x)$ so that any function $f(x)$ can be written as

$$f(x) = \sum_{n=0}^{\infty} c_n \hat{\phi}_n(x),$$

where $c_n = \langle \hat{\phi}_n | f\rangle$. Bessel's inequality then states that

$$\langle f|f\rangle \geq \sum_n |c_n|^2. \tag{17.14}$$

The equality holds if the summation is over all the basis functions. If some values of n are omitted from the sum then the inequality results (unless, of course, the c_n happen to be zero for all values of n omitted, in which case the equality remains).

17.2 Adjoint, self-adjoint and Hermitian operators

Having discussed general sets of functions, we now return to the discussion of eigenfunctions of linear operators. We begin by introducing the *adjoint* of an operator $\mathcal{L}$, denoted by $\mathcal{L}^\dagger$, which is defined by

$$\int_a^b f^*(x)\,[\mathcal{L}g(x)]\;dx = \int_a^b [\mathcal{L}^\dagger f(x)]^* g(x)\,dx + \text{boundary terms}, \tag{17.15}$$

where the boundary terms are evaluated at the end-points of the interval $[a,b]$. Thus, for any given linear differential operator $\mathcal{L}$, the adjoint operator $\mathcal{L}^\dagger$ can be found by repeated integration by parts.

An operator is said to be *self-adjoint* if $\mathcal{L}^\dagger = \mathcal{L}$. If, in addition, certain boundary conditions are met by the functions f and g on which a self-adjoint operator acts, or by the operator itself, such that the boundary terms in (17.15) vanish, then the operator is said to be *Hermitian* over the interval $a \le x \le b$. Thus, in this case,

$$\int_a^b f^*(x)\,[\mathcal{L}g(x)]\,dx = \int_a^b [\mathcal{L}f(x)]^* g(x)\,dx. \tag{17.16}$$

A little careful study will reveal the similarity between the definition of an Hermitian operator and the definition of an Hermitian matrix given in chapter 8.

►*Show that the linear operator $\mathcal{L} = d^2/dt^2$ is self-adjoint, and determine the required boundary conditions for the operator to be Hermitian over the interval t_0 to $t_0 + T$.*

Substituting into the LHS of the definition of the adjoint operator (17.15) and integrating by parts gives

$$\int_{t_0}^{t_0+T} f^* \frac{d^2 g}{dt^2}\,dt = \left[f^* \frac{dg}{dt}\right]_{t_0}^{t_0+T} - \int_{t_0}^{t_0+T} \frac{df^*}{dt}\frac{dg}{dt}\,dt.$$

Integrating the second term on the RHS by parts once more yields

$$\int_{t_0}^{t_0+T} f^* \frac{d^2 g}{dt^2}\,dt = \left[f^* \frac{dg}{dt}\right]_{t_0}^{t_0+T} + \left[-\frac{df^*}{dt}g\right]_{t_0}^{t_0+T} + \int_{t_0}^{t_0+T} g\frac{d^2 f^*}{dt^2}\,dt,$$

which, by comparison with (17.15), proves that $\mathcal{L}$ is a self-adjoint operator. Moreover, from (17.16), we see that $\mathcal{L}$ is an Hermitian operator over the required interval provided

$$\left[f^* \frac{dg}{dt}\right]_{t_0}^{t_0+T} = \left[\frac{df^*}{dt}g\right]_{t_0}^{t_0+T}. \blacktriangleleft$$

We showed in chapter 8 that the eigenvalues of Hermitian matrices are real and that their eigenvectors can be chosen to be orthogonal. Similarly, the eigenvalues of Hermitian operators are real and their eigenfunctions can be chosen to be orthogonal (we will prove these properties in the following section). Hermitian operators (or matrices) are often used in the formulation of quantum mechanics. The eigenvalues then give the possible measured values of an observable quantity such as energy or angular momentum, and the physical requirement that such quantities must be real is ensured by the reality of these eigenvalues. Furthermore, the infinite set of eigenfunctions of an Hermitian operator form a complete basis set over the relevant interval, so that it is possible to expand any function $y(x)$ obeying the appropriate conditions in an eigenfunction series over this interval:

$$y(x) = \sum_{n=0}^{\infty} c_n y_n(x), \tag{17.17}$$

where the choice of suitable values for the c_n will make the sum arbitrarily close to $y(x)$.[§] These useful properties provide the motivation for a detailed study of Hermitian operators.

§ The proof of the completeness of the eigenfunctions of an Hermitian operator is beyond the scope of this book. The reader should refer, for example, to R. Courant and D. Hilbert, *Methods of Mathematical Physics* (New York: Interscience, 1953).

17.3 Properties of Hermitian operators

We now provide proofs of some of the useful properties of Hermitian operators. Again much of the analysis is similar to that for Hermitian matrices in chapter 8, although the present section stands alone. (Here, and throughout the remainder of this chapter, we will write out inner products in full. We note, however, that the inner product notation often provides a neat form in which to express results.)

17.3.1 Reality of the eigenvalues

Consider an Hermitian operator for which (17.5) is satisfied by at least two eigenfunctions $y_i(x)$ and $y_j(x)$, which have corresponding eigenvalues λ_i and λ_j, so that

$$\mathcal{L}y_i = \lambda_i \rho(x) y_i, \tag{17.18}$$

$$\mathcal{L}y_j = \lambda_j \rho(x) y_j, \tag{17.19}$$

where we have allowed for the presence of a weight function $\rho(x)$. Multiplying (17.18) by y_j^* and (17.19) by y_i^* and then integrating gives

$$\int_a^b y_j^* \mathcal{L} y_i \, dx = \lambda_i \int_a^b y_j^* y_i \rho \, dx, \tag{17.20}$$

$$\int_a^b y_i^* \mathcal{L} y_j \, dx = \lambda_j \int_a^b y_i^* y_j \rho \, dx. \tag{17.21}$$

Remembering that we have required $\rho(x)$ to be real, the complex conjugate of (17.20) becomes

$$\int_a^b y_j (\mathcal{L} y_i)^* \, dx = \lambda_i^* \int_a^b y_i^* y_j \rho \, dx, \tag{17.22}$$

and using the definition of an Hermitian operator (17.16) it follows that the LHS of (17.22) is equal to the LHS of (17.21). Thus

$$(\lambda_i^* - \lambda_j) \int_a^b y_i^* y_j \rho \, dx = 0. \tag{17.23}$$

If $i = j$ then $\lambda_i = \lambda_i^*$ (since $\int_a^b y_i^* y_i \rho \, dx \neq 0$), which is a statement that the eigenvalue λ_i is real.

17.3.2 Orthogonality and normalisation of the eigenfunctions

From (17.23), it is immediately apparent that two eigenfunctions y_i and y_j that correspond to different eigenvalues, i.e. such that $\lambda_i \neq \lambda_j$, satisfy

$$\int_a^b y_i^* y_j \rho \, dx = 0, \tag{17.24}$$

which is a statement of the orthogonality of y_i and y_j.

If one (or more) of the eigenvalues is degenerate, however, we have different eigenfunctions corresponding to the same eigenvalue, and the proof of orthogonality is not so straightforward. Nevertheless, an orthogonal set of eigenfunctions may be constructed using the *Gram–Schmidt orthogonalisation* method mentioned earlier in this chapter and used in chapter 8 to construct a set of orthogonal eigenvectors of an Hermitian matrix. We repeat the analysis here for completeness.

Suppose, for the sake of our proof, that λ_0 is k-fold degenerate, i.e.

$$\mathcal{L}y_i = \lambda_0 \rho y_i \qquad \text{for } i = 0, 1, \ldots, k-1, \tag{17.25}$$

but that λ_0 is different from any of λ_k, λ_{k+1}, etc. Then any linear combination of these y_i is also an eigenfunction with eigenvalue λ_0 since

$$\mathcal{L}z \equiv \mathcal{L}\sum_{i=0}^{k-1} c_i y_i = \sum_{i=0}^{k-1} c_i \mathcal{L}y_i = \sum_{i=0}^{k-1} c_i \lambda_0 \rho y_i = \lambda_0 \rho z. \tag{17.26}$$

If the y_i defined in (17.25) are not already mutually orthogonal then consider the new eigenfunctions z_i constructed by the following procedure, in which each of the new functions z_i is to be normalised, to give $\hat{z}_i$, before proceeding to the construction of the next one (the normalisation can be carried out by dividing the eigenfunction z_i by $(\int_a^b z_i^* z_i \rho\, dx)^{1/2}$):

$$\begin{aligned}
z_0 &= y_0, \\
z_1 &= y_1 - \left(\hat{z}_0 \int_a^b \hat{z}_0^* y_1 \rho\, dx\right), \\
z_2 &= y_2 - \left(\hat{z}_1 \int_a^b \hat{z}_1^* y_2 \rho\, dx\right) - \left(\hat{z}_0 \int_a^b \hat{z}_0^* y_2 \rho\, dx\right), \\
&\ \vdots \\
z_{k-1} &= y_{k-1} - \left(\hat{z}_{k-2} \int_a^b \hat{z}_{k-2}^* y_{k-1} \rho\, dx\right) - \cdots - \left(\hat{z}_0 \int_a^b \hat{z}_0^* y_{k-1} \rho\, dx\right).
\end{aligned}$$

Each of the integrals is just a number and thus each new function z_i is, as can be shown from (17.26), an eigenvector of $\mathcal{L}$ with eigenvalue λ_0. It is straightforward to check that each z_i is orthogonal to all its predecessors. Thus, by this explicit construction we have shown that an orthogonal set of eigenfunctions of an Hermitian operator $\mathcal{L}$ can be obtained. Clearly the orthogonal set obtained, z_i, is not unique.

In general, since $\mathcal{L}$ is linear, the normalisation of its eigenfunctions $y_i(x)$ is arbitrary. It is often convenient, however, to work in terms of the normalised eigenfunctions $\hat{y}_i(x)$, so that $\int_a^b \hat{y}_i^* \hat{y}_i \rho\, dx = 1$. These therefore form an orthonormal set and we can write

$$\int_a^b \hat{y}_i^* \hat{y}_j \rho \, dx = \delta_{ij}, \tag{17.27}$$

which is valid for all pairs of values i, j.

17.3.3 Completeness of the eigenfunctions

As noted earlier, the eigenfunctions of an Hermitian operator may be shown to form a complete basis set over the relevant interval. One may thus expand any (reasonable) function $y(x)$ obeying appropriate boundary conditions in an eigenfunction series over the interval, as in (17.17). Working in terms of the normalised eigenfunctions $\hat{y}_n(x)$, we may thus write

$$\begin{aligned} f(x) &= \sum_n \hat{y}_n(x) \int_a^b \hat{y}_n^*(z) f(z) \rho(z) \, dz \\ &= \int_a^b f(z) \rho(z) \sum_n \hat{y}_n(x) \hat{y}_n^*(z) \, dz. \end{aligned}$$

Since this is true for any $f(x)$, we must have that

$$\rho(z) \sum_n \hat{y}_n(x) \hat{y}_n^*(z) = \delta(x - z). \tag{17.28}$$

This is called the *completeness* or *closure* property of the eigenfunctions. It defines a complete set. If the spectrum of eigenvalues of $\mathcal{L}$ is anywhere continuous then the eigenfunction $y_n(x)$ must be treated as $y(n, x)$ and an integration carried out over n.

We also note that the RHS of (17.28) is a δ-function and so is only non-zero when $z = x$; thus $\rho(z)$ on the LHS can be replaced by $\rho(x)$ if required, i.e.

$$\rho(z) \sum_n \hat{y}_n(x) \hat{y}_n^*(z) = \rho(x) \sum_n \hat{y}_n(x) \hat{y}_n^*(z). \tag{17.29}$$

17.3.4 Construction of real eigenfunctions

Recall that the eigenfunction y_i satisfies

$$\mathcal{L} y_i = \lambda_i \rho y_i \tag{17.30}$$

and that the complex conjugate of this gives

$$\mathcal{L} y_i^* = \lambda_i^* \rho y_i^* = \lambda_i \rho y_i^*, \tag{17.31}$$

where the last equality follows because the eigenvalues are real, i.e. $\lambda_i = \lambda_i^*$. Thus, y_i and y_i^* are eigenfunctions corresponding to the same eigenvalue and hence, because of the linearity of $\mathcal{L}$, at least one of $y_i^* + y_i$ and $i(y_i^* - y_i)$, which are both real, is a non-zero eigenfunction corresponding to that eigenvalue. It follows that the eigenfunctions can always be made real by taking suitable linear combinations, though taking such linear combinations will only be necessary in cases where a particular λ is degenerate, i.e. corresponds to more than one linearly independent eigenfunction.

17.4 Sturm–Liouville equations

One of the most important applications of our discussion of Hermitian operators is to the study of *Sturm–Liouville equations*, which take the general form

$$p(x)\frac{d^2y}{dx^2} + r(x)\frac{dy}{dx} + q(x)y + \lambda\rho(x)y = 0, \qquad \text{where } r(x) = \frac{dp(x)}{dx} \tag{17.32}$$

and p, q and r are real functions of x.[§] A variational approach to the Sturm–Liouville equation, which is useful in estimating the eigenvalues λ for a given set of boundary conditions on y, is discussed in chapter 22. For now, however, we concentrate on demonstrating that solutions of the Sturm–Liouville equation that satisfy appropriate boundary conditions are the eigenfunctions of an Hermitian operator.

It is clear that (17.32) can be written

$$\mathcal{L}y = \lambda\rho(x)y, \qquad \text{where } \mathcal{L} \equiv -\left[p(x)\frac{d^2}{dx^2} + r(x)\frac{d}{dx} + q(x)\right]. \tag{17.33}$$

Using the condition that $r(x) = p'(x)$, it will be seen that the general Sturm–Liouville equation (17.32) can also be rewritten as

$$(py')' + qy + \lambda\rho y = 0, \tag{17.34}$$

where primes denote differentiation with respect to x. Using (17.33) this may also be written $\mathcal{L}y \equiv -(py')' - qy = \lambda\rho y$, which defines a more useful form for the Sturm–Liouville linear operator, namely

$$\mathcal{L} \equiv -\left[\frac{d}{dx}\left(p(x)\frac{d}{dx}\right) + q(x)\right]. \tag{17.35}$$

17.4.1 Hermitian nature of the Sturm–Liouville operator

As we now show, the linear operator of the Sturm–Liouville equation (17.35) is self-adjoint. Moreover, the operator is Hermitian over the range $[a, b]$ provided

[§] We note that sign conventions vary in this expression for the general Sturm–Liouville equation; some authors use $-\lambda\rho(x)y$ on the LHS of (17.32).

certain boundary conditions are met, namely that any two eigenfunctions y_i and y_j of (17.33) must satisfy

$$\left[y_i^* p y_j'\right]_{x=a} = \left[y_i^* p y_j'\right]_{x=b} \qquad \text{for all } i, j. \tag{17.36}$$

Rearranging (17.36), we can write

$$\left[y_i^* p y_j'\right]_{x=a}^{x=b} = 0 \tag{17.37}$$

as an equivalent statement of the required boundary conditions. These boundary conditions are in fact not too restrictive and are met, for instance, by the sets $y(a) = y(b) = 0$; $y(a) = y'(b) = 0$; $p(a) = p(b) = 0$ and by many other sets. It is important to note that in order to satisfy (17.36) and (17.37) one boundary condition must be specified at each end of the range.

►*Prove that the Sturm–Liouville operator is Hermitian over the range* $[a, b]$ *and under the boundary conditions (17.37).*

Putting the Sturm–Liouville form $\mathcal{L}y = -(py')' - qy$ into the definition (17.16) of an Hermitian operator, the LHS may be written as a sum of two terms, i.e.

$$-\int_a^b \left[y_i^*(py_j')' + y_i^* q y_j\right] dx = -\int_a^b y_i^*(py_j')'\, dx - \int_a^b y_i^* q y_j\, dx.$$

The first term may be integrated by parts to give

$$-\left[y_i^* p y_j'\right]_a^b + \int_a^b (y_i^*)' p y_j'\, dx.$$

The boundary-value term in this is zero because of the boundary conditions, and so integrating by parts again yields

$$\left[(y_i^*)' p y_j\right]_a^b - \int_a^b ((y_i^*)' p)' y_j\, dx.$$

Again, the boundary-value term is zero, leaving us with

$$-\int_a^b \left[y_i^*(py_j')' + y_i^* q y_j\right] dx = -\int_a^b \left[y_j(p(y_i^*)')' + y_j q y_i^*\right] dx,$$

which proves that the Sturm–Liouville operator is Hermitian over the prescribed interval. ◄

It is also worth noting that, since $p(a) = p(b) = 0$ is a valid set of boundary conditions, many Sturm–Liouville equations possess a 'natural' interval $[a, b]$ over which the corresponding differential operator $\mathcal{L}$ is Hermitian *irrespective* of the boundary conditions satisfied by its eigenfunctions at $x = a$ and $x = b$ (the only requirement being that they are regular at these end-points).

17.4.2 Transforming an equation into Sturm–Liouville form

Many of the second-order differential equations encountered in physical problems are examples of the Sturm–Liouville equation (17.34). Moreover, *any* second-order

Equation	$p(x)$	$q(x)$	λ	$\rho(x)$
Hypergeometric	$x^c(1-x)^{a+b-c+1}$	0	$-ab$	$x^{c-1}(1-x)^{a+b-c}$
Legendre	$1-x^2$	0	$\ell(\ell+1)$	1
Associated Legendre	$1-x^2$	$-m^2/(1-x^2)$	$\ell(\ell+1)$	1
Chebyshev	$(1-x^2)^{1/2}$	0	ν^2	$(1-x^2)^{-1/2}$
Confluent hypergeometric	$x^c e^{-x}$	0	$-a$	$x^{c-1}e^{-x}$
Bessel*	x	$-\nu^2/x$	α^2	x
Laguerre	xe^{-x}	0	ν	e^{-x}
Associated Laguerre	$x^{m+1}e^{-x}$	0	ν	$x^m e^{-x}$
Hermite	e^{-x^2}	0	2ν	e^{-x^2}
Simple harmonic	1	0	ω^2	1

Table 17.1 The Sturm–Liouville form (17.34) for important ODEs in the physical sciences and engineering. The asterisk denotes that, for Bessel's equation, a change of variable $x \to x/a$ is required to give the conventional normalisation used here, but is not needed for the transformation into Sturm–Liouville form.

differential equation of the form

$$p(x)y'' + r(x)y' + q(x)y + \lambda\rho(x)y = 0 \tag{17.38}$$

can be converted into Sturm–Liouville form by multiplying through by a suitable integrating factor, which is given by

$$F(x) = \exp\left\{\int^x \frac{r(u) - p'(u)}{p(u)}\, du\right\}. \tag{17.39}$$

It is easily verified that (17.38) then takes the Sturm–Liouville form,

$$[F(x)p(x)y']' + F(x)q(x)y + \lambda F(x)\rho(x)y = 0, \tag{17.40}$$

with a different, but still non-negative, weight function $F(x)\rho(x)$. Table 17.1 summarises the Sturm–Liouville form (17.34) for several of the equations listed in table 16.1. These forms can be determined using (17.39), as illustrated in the following example.

►*Put the following equations into Sturm–Liouville (SL) form:*

(i) $(1-x^2)y'' - xy' + \nu^2 y = 0$ *(Chebyshev equation)*;

(ii) $xy'' + (1-x)y' + \nu y = 0$ *(Laguerre equation)*;

(iii) $y'' - 2xy' + 2\nu y = 0$ *(Hermite equation)*.

(i) From (17.39), the required integrating factor is

$$F(x) = \exp\left(\int^x \frac{u}{1-u^2}\, du\right) = \exp\left[-\tfrac{1}{2}\ln(1-x^2)\right] = (1-x^2)^{-1/2}.$$

Thus, the Chebyshev equation becomes

$$(1-x^2)^{1/2}y'' - x(1-x^2)^{-1/2}y' + \nu^2(1-x^2)^{-1/2}y = \left[(1-x^2)^{1/2}y'\right]' + \nu^2(1-x^2)^{-1/2}y = 0,$$

which is in SL form with $p(x) = (1-x^2)^{1/2}$, $q(x) = 0$, $\rho(x) = (1-x^2)^{-1/2}$ and $\lambda = \nu^2$.

(ii) From (17.39), the required integrating factor is

$$F(x) = \exp\left(\int^x -1\,du\right) = \exp(-x).$$

Thus, the Laguerre equation becomes

$$xe^{-x}y'' + (1-x)e^{-x}y' + \nu e^{-x}y = (xe^{-x}y')' + \nu e^{-x}y = 0,$$

which is in SL form with $p(x) = xe^{-x}$, $q(x) = 0$, $\rho(x) = e^{-x}$ and $\lambda = \nu$.

(iii) From (17.39), the required integrating factor is

$$F(x) = \exp\left(\int^x -2u\,du\right) = \exp(-x^2).$$

Thus, the Hermite equation becomes

$$e^{-x^2}y'' - 2xe^{-x^2}y' + 2\nu e^{-x^2}y = (e^{-x^2}y')' + 2\nu e^{-x^2}y = 0,$$

which is in SL form with $p(x) = e^{-x^2}$, $q(x) = 0$, $\rho(x) = e^{-x^2}$ and $\lambda = 2\nu$. ◄

From the $p(x)$ entries in table 17.1, we may read off the natural interval over which the corresponding Sturm–Liouville operator (17.35) is Hermitian; in each case this is given by $[a, b]$, where $p(a) = p(b) = 0$. Thus, the natural interval for the Legendre equation, the associated Legendre equation and the Chebyshev equation is $[-1, 1]$; for the Laguerre and associated Laguerre equations the interval is $[0, \infty]$; and for the Hermite equation it is $[-\infty, \infty]$. In addition, from (17.37), one sees that for the simple harmonic equation one requires only that $[a, b] = [x_0, x_0 + 2\pi]$. We also note that, as required, the weight function in each case is finite and non-negative over the natural interval. Occasionally, a little more care is required when determining the conditions for a Sturm–Liouville operator of the form (17.35) to be Hermitian over some natural interval, as is illustrated in the following example.

►*Express the hypergeometric equation,*

$$x(1-x)y'' + [\,c - (a+b+1)x\,]y' - aby = 0,$$

in Sturm–Liouville form. Hence determine the natural interval over which the resulting Sturm–Liouville operator is Hermitian and the corresponding conditions that one must impose on the parameters a, b and c.

As usual for an equation not already in SL form, we first determine the appropriate integrating factor. This is given, as in equation (17.39), by

$$
\begin{aligned}
F(x) &= \exp\left[\int^x \frac{c-(a+b+1)u-1+2u}{u(1-u)}\,du\right] \\
&= \exp\left[\int^x \frac{c-1-(a+b-1)u}{u(1-u)}\,du\right] \\
&= \exp\left[\int^x \left(\frac{c-1}{1-u}+\frac{c-1}{u}-\frac{a+b-1}{1-u}\,du\right)\right] \\
&= \exp\left[(a+b-c)\ln(1-x)+(c-1)\ln x\right] \\
&= x^{c-1}(1-x)^{a+b-c}.
\end{aligned}
$$

When the equation is multiplied through by $F(x)$ it takes the form

$$\left[x^c(1-x)^{a+b-c+1}y'\right]' - abx^{c-1}(1-x)^{a+b-c}y = 0.$$

Now, for the corresponding Sturm–Liouville operator to be Hermitian, the conditions to be imposed are as follows.

(i) The boundary condition (17.37); if $c > 0$ and $a+b-c+1 > 0$, this is satisfied automatically for $0 \leq x \leq 1$, which is thus the natural interval in this case.
(ii) The weight function $x^{c-1}(1-x)^{a+b-c}$ must be finite and not change sign in the interval $0 \leq x \leq 1$. This means that both exponents in it must be positive, i.e. $c-1 > 0$ and $a+b-c > 0$.

Putting together the conditions on the parameters gives the double inequality $a+b > c > 1$. ◄

Finally, we consider Bessel's equation,

$$x^2y'' + xy' + (x^2-\nu^2)y = 0,$$

which may be converted into Sturm–Liouville form, but only in a somewhat unorthodox fashion. It is conventional first to divide the Bessel equation by x and then to change variables to $\bar{x} = x/\alpha$. In this case, it becomes

$$\bar{x}y''(\alpha\bar{x}) + y'(\alpha\bar{x}) - \frac{\nu^2}{\bar{x}}y(\alpha\bar{x}) + \alpha^2\bar{x}y(\alpha\bar{x}) = 0, \qquad (17.41)$$

where a prime now indicates differentiation with respect to $\bar{x}$. Dropping the bars on the independent variable, we thus have

$$[xy'(\alpha x)]' - \frac{\nu^2}{x}y(\alpha x) + \alpha^2 xy(\alpha x) = 0, \qquad (17.42)$$

which is in SL form with $p(x) = x$, $q(x) = -\nu^2/x$, $\rho(x) = x$ and $\lambda = \alpha^2$. It should be noted, however, that in this case the eigenvalue (actually its square root) appears in the argument of the dependent variable.

17.5 Superposition of eigenfunctions: Green's functions

We have already seen that if

$$\mathcal{L}y_n(x) = \lambda_n \rho(x) y_n(x), \tag{17.43}$$

where $\mathcal{L}$ is an Hermitian operator, then the eigenvalues λ_n are real and the eigenfunctions $y_n(x)$ are orthogonal (or can be made so). Let us assume that we know the eigenfunctions $y_n(x)$ of $\mathcal{L}$ that individually satisfy (17.43) and some imposed boundary conditions (for which $\mathcal{L}$ is Hermitian).

Now let us suppose we wish to solve the inhomogeneous differential equation

$$\mathcal{L}y(x) = f(x), \tag{17.44}$$

subject to the same boundary conditions. Since the eigenfunctions of $\mathcal{L}$ form a complete set, the full solution, $y(x)$, to (17.44) may be written as a superposition of eigenfunctions, i.e.

$$y(x) = \sum_{n=0}^{\infty} c_n y_n(x), \tag{17.45}$$

for some choice of the constants c_n. Making full use of the linearity of $\mathcal{L}$, we have

$$f(x) = \mathcal{L}y(x) = \mathcal{L}\left(\sum_{n=0}^{\infty} c_n y_n(x)\right) = \sum_{n=0}^{\infty} c_n \mathcal{L}y_n(x) = \sum_{n=0}^{\infty} c_n \lambda_n \rho(x) y_n(x). \tag{17.46}$$

Multiplying the first and last terms of (17.46) by y_j^* and integrating, we obtain

$$\int_a^b y_j^*(z) f(z)\, dz = \sum_{n=0}^{\infty} \int_a^b c_n \lambda_n y_j^*(z) y_n(z) \rho(z)\, dz, \tag{17.47}$$

where we have used z as the integration variable for later convenience. Finally, using the orthogonality condition (17.27), we see that the integrals on the RHS are zero unless $n = j$, and so obtain

$$c_n = \frac{1}{\lambda_n} \frac{\int_a^b y_n^*(z) f(z)\, dz}{\int_a^b y_n^*(z) y_n(z) \rho(z)\, dz}. \tag{17.48}$$

Thus, if we can find all the eigenfunctions of a differential operator then (17.48) can be used to find the weighting coefficients for the superposition, to give as the full solution

$$y(x) = \sum_{n=0}^{\infty} \frac{1}{\lambda_n} \frac{\int_a^b y_n^*(z) f(z)\, dz}{\int_a^b y_n^*(z) y_n(z) \rho(z)\, dz}\, y_n(x). \tag{17.49}$$

If we work with normalised eigenfunctions $\hat{y}_n(x)$, so that

$$\int_a^b \hat{y}_n^*(z) \hat{y}_n(z) \rho(z)\, dz = 1 \qquad \text{for all } n,$$

and we assume that we may interchange the order of summation and integration, then (17.49) can be written as

$$y(x) = \int_a^b \left\{ \sum_{n=0}^{\infty} \left[\frac{1}{\lambda_n} \hat{y}_n(x) \hat{y}_n^*(z) \right] \right\} f(z)\, dz.$$

The quantity in braces, which is a function of x and z only, is usually written $G(x, z)$, and is the *Green's function* for the problem. With this notation,

$$y(x) = \int_a^b G(x, z) f(z)\, dz, \tag{17.50}$$

where

$$G(x, z) = \sum_{n=0}^{\infty} \frac{1}{\lambda_n} \hat{y}_n(x) \hat{y}_n^*(z). \tag{17.51}$$

We note that $G(x, z)$ is determined entirely by the boundary conditions and the eigenfunctions $\hat{y}_n$, and hence by $\mathcal{L}$ itself, and that $f(z)$ depends purely on the RHS of the inhomogeneous equation (17.44). Thus, for a given $\mathcal{L}$ and boundary conditions we can establish, once and for all, a function $G(x, z)$ that will enable us to solve the inhomogeneous equation for *any* RHS. From (17.51) we also note that

$$G(x, z) = G^*(z, x). \tag{17.52}$$

We have already met the Green's function in the solution of second-order differential equations in chapter 15, as the function that satisfies the equation $\mathcal{L}[G(x, z)] = \delta(x - z)$ (and the boundary conditions). The formulation given above is an alternative, though equivalent, one.

►*Find an appropriate Green's function for the equation*

$$y'' + \tfrac{1}{4} y = f(x),$$

with boundary conditions $y(0) = y(\pi) = 0$. *Hence, solve for* (i) $f(x) = \sin 2x$ *and* (ii) $f(x) = x/2$.

One approach to solving this problem is to use the methods of chapter 15 and find a complementary function and particular integral. However, in order to illustrate the techniques developed in the present chapter we will use the superposition of eigenfunctions, which, as may easily be checked, produces the same solution.

The operator on the LHS of this equation is already Hermitian under the given boundary conditions, and so we seek its eigenfunctions. These satisfy the equation

$$y'' + \tfrac{1}{4} y = \lambda y.$$

This equation has the familiar solution

$$y(x) = A \sin\left(\sqrt{\tfrac{1}{4} - \lambda}\right) x + B \cos\left(\sqrt{\tfrac{1}{4} - \lambda}\right) x.$$

Now, the boundary conditions require that $B = 0$ and $\sin\left(\sqrt{\frac{1}{4} - \lambda}\right)\pi = 0$, and so

$$\sqrt{\tfrac{1}{4} - \lambda} = n, \qquad \text{where } n = 0, \pm 1, \pm 2, \ldots.$$

Therefore, the independent eigenfunctions that satisfy the boundary conditions are

$$y_n(x) = A_n \sin nx,$$

where n is any non-negative integer, and the corresponding eigenvalues are $\lambda_n = \frac{1}{4} - n^2$. The normalisation condition further requires

$$\int_0^\pi A_n^2 \sin^2 nx \, dx = 1 \qquad \Rightarrow \qquad A_n = \left(\frac{2}{\pi}\right)^{1/2}.$$

Comparison with (17.51) shows that the appropriate Green's function is therefore given by

$$G(x, z) = \frac{2}{\pi} \sum_{n=0}^{\infty} \frac{\sin nx \sin nz}{\frac{1}{4} - n^2}.$$

Case (i). Using (17.50), the solution with $f(x) = \sin 2x$ is given by

$$y(x) = \frac{2}{\pi} \int_0^\pi \left(\sum_{n=0}^{\infty} \frac{\sin nx \sin nz}{\frac{1}{4} - n^2} \right) \sin 2z \, dz = \frac{2}{\pi} \sum_{n=0}^{\infty} \frac{\sin nx}{\frac{1}{4} - n^2} \int_0^\pi \sin nz \sin 2z \, dz.$$

Now the integral is zero unless $n = 2$, in which case it is

$$\int_0^\pi \sin^2 2z \, dz = \frac{\pi}{2}.$$

Thus

$$y(x) = -\frac{2}{\pi} \frac{\sin 2x}{15/4} \frac{\pi}{2} = -\frac{4}{15} \sin 2x$$

is the full solution for $f(x) = \sin 2x$. This is, of course, exactly the solution found by using the methods of chapter 15.

Case (ii). The solution with $f(x) = x/2$ is given by

$$y(x) = \int_0^\pi \left(\frac{2}{\pi} \sum_{n=0}^{\infty} \frac{\sin nx \sin nz}{\frac{1}{4} - n^2} \right) \frac{z}{2} \, dz = \frac{1}{\pi} \sum_{n=0}^{\infty} \frac{\sin nx}{\frac{1}{4} - n^2} \int_0^\pi z \sin nz \, dz.$$

The integral may be evaluated by integrating by parts. For $n \neq 0$,

$$\begin{aligned} \int_0^\pi z \sin nz \, dz &= \left[-\frac{z \cos nz}{n} \right]_0^\pi + \int_0^\pi \frac{\cos nz}{n} \, dz \\ &= \frac{-\pi \cos n\pi}{n} + \left[\frac{\sin nz}{n^2} \right]_0^\pi \\ &= -\frac{\pi(-1)^n}{n}. \end{aligned}$$

For $n = 0$ the integral is zero, and thus

$$y(x) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{\sin nx}{n\left(\frac{1}{4} - n^2\right)},$$

is the full solution for $f(x) = x/2$. Using the methods of subsection 15.1.2, the solution is found to be $y(x) = 2x - 2\pi \sin(x/2)$, which may be shown to be equal to the above solution by expanding $2x - 2\pi \sin(x/2)$ as a Fourier sine series. ◄

17.6 A useful generalisation

Sometimes we encounter inhomogeneous equations of a form slightly more general than (17.1), given by

$$\mathcal{L}y(x) - \mu\rho(x)y(x) = f(x) \tag{17.53}$$

for some Hermitian operator $\mathcal{L}$, with y subject to the appropriate boundary conditions and μ a given (i.e. *fixed*) constant. To solve this equation we expand $y(x)$ and $f(x)$ in terms of the eigenfunctions $y_n(x)$ of the operator $\mathcal{L}$, which satisfy

$$\mathcal{L}y_n(x) = \lambda_n\rho(x)y_n(x).$$

Working in terms of the normalised eigenfunctions $\hat{y}_n(x)$, we first expand $f(x)$ as follows:

$$\begin{aligned} f(x) &= \sum_{n=0}^{\infty}\hat{y}_n(x)\int_a^b \hat{y}_n^*(z)f(z)\rho(z)\,dz \\ &= \int_a^b \rho(z)\sum_{n=0}^{\infty}\hat{y}_n(x)\hat{y}_n^*(z)f(z)\,dz. \end{aligned} \tag{17.54}$$

Using (17.29) this becomes

$$\begin{aligned} f(x) &= \int_a^b \rho(x)\sum_{n=0}^{\infty}\hat{y}_n(x)\hat{y}_n^*(z)f(z)\,dz \\ &= \rho(x)\sum_{n=0}^{\infty}\hat{y}_n(x)\int_a^b \hat{y}_n^*(z)f(z)\,dz. \end{aligned} \tag{17.55}$$

Next, we expand $y(x)$ as $y = \sum_{n=0}^{\infty} c_n\hat{y}_n(x)$ and seek the coefficients c_n. Substituting this and (17.55) into (17.53) we have

$$\rho(x)\sum_{n=0}^{\infty}(\lambda_n - \mu)c_n\hat{y}_n(x) = \rho(x)\sum_{n=0}^{\infty}\hat{y}_n(x)\int_a^b \hat{y}_n^*(z)f(z)\,dz,$$

from which we find that

$$c_n = \sum_{n=0}^{\infty}\frac{\int_a^b \hat{y}_n^*(z)f(z)\,dz}{\lambda_n - \mu}.$$

Hence the solution of (17.53) is given by

$$y = \sum_{n=0}^{\infty} c_n\hat{y}_n(x) = \sum_{n=0}^{\infty}\frac{\hat{y}_n(x)}{\lambda_n - \mu}\int_a^b \hat{y}_n^*(z)f(z)\,dz = \int_a^b\sum_{n=0}^{\infty}\frac{\hat{y}_n(x)\hat{y}_n^*(z)}{\lambda_n - \mu}f(z)\,dz.$$

From this we may identify the Green's function

$$G(x,z) = \sum_{n=0}^{\infty}\frac{\hat{y}_n(x)\hat{y}_n^*(z)}{\lambda_n - \mu}.$$

We note that if $\mu = \lambda_n$, i.e. if μ equals one of the eigenvalues of $\mathcal{L}$, then $G(x, z)$ becomes infinite and this method runs into difficulty. No solution then exists unless the RHS of (17.53) satisfies the relation

$$\int_a^b \hat{y}_n^*(x) f(x)\, dx = 0.$$

If the spectrum of eigenvalues of the operator $\mathcal{L}$ is anywhere continuous, the orthonormality and closure relationships of the normalised eigenfunctions become

$$\int_a^b \hat{y}_n^*(x)\hat{y}_m(x)\rho(x)\, dx = \delta(n-m),$$
$$\int_0^\infty \hat{y}_n^*(z)\hat{y}_n(x)\rho(x)\, dn = \delta(x-z).$$

Repeating the above analysis we then find that the Green's function is given by

$$G(x, z) = \int_0^\infty \frac{\hat{y}_n(x)\hat{y}_n^*(z)}{\lambda_n - \mu}\, dn.$$

17.7 Exercises

17.1 By considering $\langle h|h\rangle$, where $h = f + \lambda g$ with λ real, prove that, for two functions f and g,

$$\langle f|f\rangle\langle g|g\rangle \geq \tfrac{1}{4}[\langle f|g\rangle + \langle g|f\rangle]^2.$$

The function $y(x)$ is real and positive for all x. Its Fourier cosine transform $\tilde{y}_c(k)$ is defined by

$$\tilde{y}_c(k) = \int_{-\infty}^{\infty} y(x)\cos(kx)\, dx,$$

and it is given that $\tilde{y}_c(0) = 1$. Prove that

$$\tilde{y}_c(2k) \geq 2[\tilde{y}_c(k)]^2 - 1.$$

17.2 Write the homogeneous Sturm-Liouville eigenvalue equation for which $y(a) = y(b) = 0$ as

$$\mathscr{L}(y; \lambda) \equiv (py')' + qy + \lambda\rho y = 0,$$

where $p(x), q(x)$ and $\rho(x)$ are continuously differentiable functions. Show that if $z(x)$ and $F(x)$ satisfy $\mathcal{L}(z; \lambda) = F(x)$, with $z(a) = z(b) = 0$, then

$$\int_a^b y(x)F(x)\, dx = 0.$$

Demonstrate the validity of this general result by direct calculation for the specific case in which $p(x) = \rho(x) = 1$, $q(x) = 0$, $a = -1$, $b = 1$ and $z(x) = 1 - x^2$.

17.3 Consider the real eigenfunctions $y_n(x)$ of a Sturm–Liouville equation,

$$(py')' + qy + \lambda\rho y = 0, \qquad a \leq x \leq b,$$

in which $p(x)$, $q(x)$ and $\rho(x)$ are continuously differentiable real functions and $p(x)$ does not change sign in $a \leq x \leq b$. Take $p(x)$ as positive throughout the interval, if necessary by changing the signs of all eigenvalues. For $a \leq x_1 \leq x_2 \leq b$, establish the identity

$$(\lambda_n - \lambda_m) \int_{x_1}^{x_2} \rho y_n y_m \, dx = \left[y_n \, p \, y_m' - y_m \, p \, y_n' \right]_{x_1}^{x_2}.$$

Deduce that if $\lambda_n > \lambda_m$ then $y_n(x)$ must change sign between two successive zeros of $y_m(x)$.
[The reader may find it helpful to illustrate this result by sketching the first few eigenfunctions of the system $y'' + \lambda y = 0$, with $y(0) = y(\pi) = 0$, and the Legendre polynomials $P_n(z)$ for $n = 2, 3, 4, 5$.]

17.4 Show that the equation

$$y'' + a\delta(x)y + \lambda y = 0,$$

with $y(\pm\pi) = 0$ and a real, has a set of eigenvalues λ satisfying

$$\tan(\pi\sqrt{\lambda}) = \frac{2\sqrt{\lambda}}{a}.$$

Investigate the conditions under which negative eigenvalues, $\lambda = -\mu^2$, with μ real, are possible.

17.5 Use the properties of Legendre polynomials to carry out the following exercises.

(a) Find the solution of $(1 - x^2)y'' - 2xy' + by = f(x)$, valid in the range $-1 \leq x \leq 1$ and finite at $x = 0$, in terms of Legendre polynomials.
(b) If $b = 14$ and $f(x) = 5x^3$, find the explicit solution and verify it by direct substitution.

[The first six Legendre polynomials are listed in Subsection 18.1.1.]

17.6 Starting from the linearly independent functions $1, x, x^2, x^3, \ldots$, in the range $0 \leq x < \infty$, find the first three orthogonal functions ϕ_0, ϕ_1 and ϕ_2, with respect to the weight function $\rho(x) = e^{-x}$. By comparing your answers with the Laguerre polynomials generated by the recurrence relation (18.115), deduce the form of $\phi_3(x)$.

17.7 Consider the set of functions, $\{f(x)\}$, of the real variable x, defined in the interval $-\infty < x < \infty$, that $\to 0$ at least as quickly as x^{-1} as $x \to \pm\infty$. For unit weight function, determine whether each of the following linear operators is Hermitian when acting upon $\{f(x)\}$:

$$\text{(a)}\ \frac{d}{dx} + x; \quad \text{(b)}\ -i\frac{d}{dx} + x^2; \quad \text{(c)}\ ix\frac{d}{dx}; \quad \text{(d)}\ i\frac{d^3}{dx^3}.$$

17.8 A particle moves in a parabolic potential in which its natural angular frequency of oscillation is $\frac{1}{2}$. At time $t = 0$ it passes through the origin with velocity v. It is then suddenly subjected to an additional acceleration, of $+1$ for $0 \leq t \leq \pi/2$, followed by -1 for $\pi/2 < t \leq \pi$. At the end of this period it is again at the origin. Apply the results of the worked example in section 17.5 to show that

$$v = -\frac{8}{\pi} \sum_{m=0}^{\infty} \frac{1}{(4m+2)^2 - \frac{1}{4}} \approx -0.81.$$

17.9 Find an eigenfunction expansion for the solution, with boundary conditions $y(0) = y(\pi) = 0$, of the inhomogeneous equation

$$\frac{d^2y}{dx^2} + \kappa y = f(x),$$

where κ is a constant and

$$f(x) = \begin{cases} x & 0 \le x \le \pi/2, \\ \pi - x & \pi/2 < x \le \pi. \end{cases}$$

17.10 Consider the following two approaches to constructing a Green's function.

(a) Find those eigenfunctions $y_n(x)$ of the self-adjoint linear differential operator d^2/dx^2 that satisfy the boundary conditions $y_n(0) = y_n(\pi) = 0$, and hence construct its Green's function $G(x, z)$.

(b) Construct the same Green's function using a method based on the complementary function of the appropriate differential equation and the boundary conditions to be satisfied at the position of the δ-function, showing that it is

$$G(x, z) = \begin{cases} x(z - \pi)/\pi & 0 \le x \le z, \\ z(x - \pi)/\pi & z \le x \le \pi. \end{cases}$$

(c) By expanding the function given in (b) in terms of the eigenfunctions $y_n(x)$, verify that it is the same function as that derived in (a).

17.11 The differential operator $\mathcal{L}$ is defined by

$$\mathcal{L}y = -\frac{d}{dx}\left(e^x \frac{dy}{dx}\right) - \tfrac{1}{4}e^x y.$$

Determine the eigenvalues λ_n of the problem

$$\mathcal{L}y_n = \lambda_n e^x y_n \qquad 0 < x < 1,$$

with boundary conditions

$$y(0) = 0, \qquad \frac{dy}{dx} + \tfrac{1}{2}y = 0 \quad \text{at} \quad x = 1.$$

(a) Find the corresponding unnormalised y_n, and also a weight function $\rho(x)$ with respect to which the y_n are orthogonal. Hence, select a suitable normalisation for the y_n.

(b) By making an eigenfunction expansion, solve the equation

$$\mathcal{L}y = -e^{x/2}, \qquad 0 < x < 1,$$

subject to the same boundary conditions as previously.

17.12 Show that the linear operator

$$\mathcal{L} \equiv \tfrac{1}{4}(1 + x^2)^2 \frac{d^2}{dx^2} + \tfrac{1}{2}x(1 + x^2)\frac{d}{dx} + a,$$

acting upon functions defined in $-1 \le x \le 1$ and vanishing at the end-points of the interval, is Hermitian with respect to the weight function $(1 + x^2)^{-1}$.

By making the change of variable $x = \tan(\theta/2)$, find two even eigenfunctions, $f_1(x)$ and $f_2(x)$, of the differential equation

$$\mathcal{L}u = \lambda u.$$

17.13 By substituting $x = \exp t$, find the normalised eigenfunctions $y_n(x)$ and the eigenvalues λ_n of the operator $\mathcal{L}$ defined by

$$\mathcal{L}y = x^2 y'' + 2xy' + \tfrac{1}{4}y, \qquad 1 \le x \le e,$$

with $y(1) = y(e) = 0$. Find, as a series $\sum a_n y_n(x)$, the solution of $\mathcal{L}y = x^{-1/2}$.

17.14 Express the solution of Poisson's equation in electrostatics,

$$\nabla^2\phi(\mathbf{r}) = -\rho(\mathbf{r})/\epsilon_0,$$

where ρ is the non-zero charge density over a finite part of space, in the form of an integral and hence identify the Green's function for the ∇^2 operator.

17.15 In the quantum-mechanical study of the scattering of a particle by a potential, a Born-approximation solution can be obtained in terms of a function $y(\mathbf{r})$ that satisfies an equation of the form

$$(-\nabla^2 - K^2)y(\mathbf{r}) = F(\mathbf{r}).$$

Assuming that $y_{\mathbf{k}}(\mathbf{r}) = (2\pi)^{-3/2}\exp(i\mathbf{k}\cdot\mathbf{r})$ is a suitably normalised eigenfunction of $-\nabla^2$ corresponding to eigenvalue k^2, find a suitable Green's function $G_K(\mathbf{r},\mathbf{r}')$. By taking the direction of the vector $\mathbf{r}-\mathbf{r}'$ as the polar axis for a $\mathbf{k}$-space integration, show that $G_K(\mathbf{r},\mathbf{r}')$ can be reduced to

$$\frac{1}{4\pi^2|\mathbf{r}-\mathbf{r}'|}\int_{-\infty}^{\infty}\frac{w\sin w}{w^2-w_0^2}\,dw,$$

where $w_0 = K|\mathbf{r}-\mathbf{r}'|$.

[This integral can be evaluated using a contour integration (chapter 24) to give $(4\pi|\mathbf{r}-\mathbf{r}'|)^{-1}\exp(iK|\mathbf{r}-\mathbf{r}'|)$.]

17.8 Hints and answers

17.1 Express the condition $\langle h|h\rangle \geq 0$ as a quadratic equation in λ and then apply the condition for no real roots, noting that $\langle f|g\rangle + \langle g|f\rangle$ is real. To put a limit on $\int y\cos^2 kx\,dx$, set $f = y^{1/2}\cos kx$ and $g = y^{1/2}$ in the inequality.

17.3 Follow an argument similar to that used for proving the reality of the eigenvalues, but integrate from x_1 to x_2, rather than from a to b. Take x_1 and x_2 as two successive zeros of $y_m(x)$ and note that, if the sign of y_m is α then the sign of $y_m'(x_1)$ is α whilst that of $y_m'(x_2)$ is $-\alpha$. Now assume that $y_n(x)$ does not change sign in the interval and has a constant sign β; show that this leads to a contradiction between the signs of the two sides of the identity.

17.5 (a) $y = \sum a_n P_n(x)$ with

$$a_n = \frac{n+1/2}{b-n(n+1)}\int_{-1}^{1} f(z)P_n(z)\,dz;$$

(b) $5x^3 = 2P_3(x)+3P_1(x)$, giving $a_1 = 1/4$ and $a_3 = 1$, leading to $y = 5(2x^3-x)/4$.

17.7 (a) No, $\int gf^{*\prime}dx \neq 0$; (b) yes; (c) no, $i\int f^* g dx \neq 0$; (d) yes.

17.9 The normalised eigenfunctions are $(2/\pi)^{1/2}\sin nx$, with n an integer. $y(x) = (4/\pi)\sum_{n\text{ odd}}[(-1)^{(n-1)/2}\sin nx]/[n^2(\kappa - n^2)]$.

17.11 $\lambda_n = (n+1/2)^2\pi^2$, $n = 0, 1, 2, \ldots$.
(a) Since $y_n(1)y_m'(1) \neq 0$, the Sturm–Liouville boundary conditions are not satisfied and the appropriate weight function has to be justified by inspection. The normalised eigenfunctions are $\sqrt{2}e^{-x/2}\sin[(n+1/2)\pi x]$, with $\rho(x) = e^x$.
(b) $y(x) = (-2/\pi^3)\sum_{n=0}^{\infty} e^{-x/2}\sin[(n+1/2)\pi x]/(n+1/2)^3$.

17.13 $y_n(x) = \sqrt{2}x^{-1/2}\sin(n\pi\ln x)$ with $\lambda_n = -n^2\pi^2$;

$$a_n = \begin{cases} -(n\pi)^{-2}\int_1^e \sqrt{2}x^{-1}\sin(n\pi\ln x)\,dx = -\sqrt{8}(n\pi)^{-3} & \text{for } n \text{ odd},\\ 0 & \text{for } n \text{ even}.\end{cases}$$

17.15 Use the form of Green's function that is the integral over all eigenvalues of the 'outer product' of two eigenfunctions corresponding to the same eigenvalue, but with arguments $\mathbf{r}$ and $\mathbf{r}'$.

18

Special functions

In the previous two chapters, we introduced the most important second-order linear ODEs in physics and engineering, listing their regular and irregular singular points in table 16.1 and their Sturm–Liouville forms in table 17.1. These equations occur with such frequency that solutions to them, which obey particular commonly occurring boundary conditions, have been extensively studied and given special names. In this chapter, we discuss these so-called 'special functions' and their properties. In addition, we also discuss some special functions that are not derived from solutions of important second-order ODEs, namely the gamma function and related functions. These convenient functions appear in a number of contexts, and so in section 18.12 we gather together some of their properties, with a minimum of formal proofs.

18.1 Legendre functions

Legendre's differential equation has the form

$$(1-x^2)y'' - 2xy' + \ell(\ell+1)y = 0, \tag{18.1}$$

and has three regular singular points, at $x = -1, 1, \infty$. It occurs in numerous physical applications and particularly in problems with axial symmetry that involve the ∇^2 operator, when they are expressed in spherical polar coordinates. In normal usage the variable x in Legendre's equation is the cosine of the polar angle in spherical polars, and thus $-1 \le x \le 1$. The parameter ℓ is a given real number, and any solution of (18.1) is called a *Legendre function*.

In subsection 16.1.1, we showed that $x = 0$ is an ordinary point of (18.1), and so we expect to find two linearly independent solutions of the form $y = \sum_{n=0}^{\infty} a_n x^n$. Substituting, we find

$$\sum_{n=0}^{\infty} \left[n(n-1)a_n x^{n-2} - n(n-1)a_n x^n - 2na_n x^n + \ell(\ell+1)a_n x^n \right] = 0,$$

which on collecting terms gives

$$\sum_{n=0}^{\infty} \{(n+2)(n+1)a_{n+2} - [n(n+1) - \ell(\ell+1)]a_n\} x^n = 0.$$

The recurrence relation is therefore

$$a_{n+2} = \frac{[n(n+1) - \ell(\ell+1)]}{(n+1)(n+2)} a_n, \tag{18.2}$$

for $n = 0, 1, 2, \ldots$. If we choose $a_0 = 1$ and $a_1 = 0$ then we obtain the solution

$$y_1(x) = 1 - \ell(\ell+1)\frac{x^2}{2!} + (\ell-2)\ell(\ell+1)(\ell+3)\frac{x^4}{4!} - \cdots, \tag{18.3}$$

whereas on choosing $a_0 = 0$ and $a_1 = 1$ we find a second solution

$$y_2(x) = x - (\ell-1)(\ell+2)\frac{x^3}{3!} + (\ell-3)(\ell-1)(\ell+2)(\ell+4)\frac{x^5}{5!} - \cdots. \tag{18.4}$$

By applying the ratio test to these series (see subsection 4.3.2), we find that both series converge for $|x| < 1$, and so their radius of convergence is unity, which (as expected) is the distance to the nearest singular point of the equation. Since (18.3) contains only even powers of x and (18.4) contains only odd powers, these two solutions cannot be proportional to one another, and are therefore linearly independent. Hence, the general solution to (18.1) for $|x| < 1$ is

$$y(x) = c_1 y_1(x) + c_2 y_2(x).$$

18.1.1 Legendre functions for integer ℓ

In many physical applications the parameter ℓ in Legendre's equation (18.1) is an integer, i.e. $\ell = 0, 1, 2, \ldots$. In this case, the recurrence relation (18.2) gives

$$a_{\ell+2} = \frac{[\ell(\ell+1) - \ell(\ell+1)]}{(\ell+1)(\ell+2)} a_\ell = 0,$$

i.e. the series terminates and we obtain a polynomial solution of order ℓ. In particular, if ℓ is even, then $y_1(x)$ in (18.3) reduces to a polynomial, whereas if ℓ is odd the same is true of $y_2(x)$ in (18.4). These solutions (suitably normalised) are called the *Legendre polynomials* of order ℓ; they are written $P_\ell(x)$ and are valid for all finite x. It is conventional to normalise $P_\ell(x)$ in such a way that $P_\ell(1) = 1$, and as a consequence $P_\ell(-1) = (-1)^\ell$. The first few Legendre polynomials are easily constructed and are given by

$$P_0(x) = 1, \qquad P_1(x) = x,$$
$$P_2(x) = \tfrac{1}{2}(3x^2 - 1), \qquad P_3(x) = \tfrac{1}{2}(5x^3 - 3x),$$
$$P_4(x) = \tfrac{1}{8}(35x^4 - 30x^2 + 3), \qquad P_5(x) = \tfrac{1}{8}(63x^5 - 70x^3 + 15x).$$

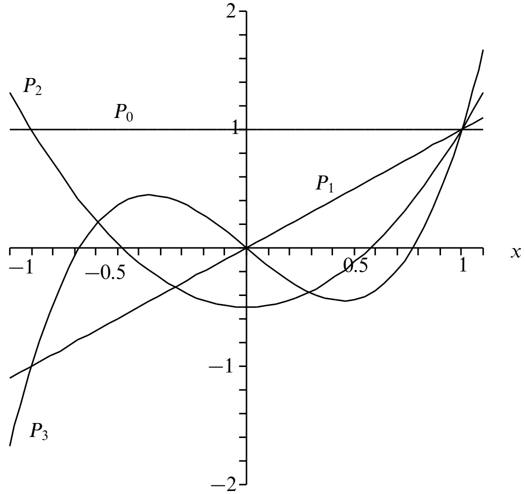

Figure 18.1 The first four Legendre polynomials.

The first four Legendre polynomials are plotted in figure 18.1.

Although, according to whether ℓ is an even or odd integer, respectively, either $y_1(x)$ in (18.3) or $y_2(x)$ in (18.4) terminates to give a multiple of the corresponding Legendre polynomial $P_\ell(x)$, the other series in each case does not terminate and therefore converges only for $|x| < 1$. According to whether ℓ is even or odd, we define *Legendre functions of the second kind* as $Q_\ell(x) = \alpha_\ell y_2(x)$ or $Q_\ell(x) = \beta_\ell y_1(x)$, respectively, where the constants α_ℓ and β_ℓ are conventionally taken to have the values

$$\alpha_\ell = \frac{(-1)^{\ell/2} 2^\ell [(\ell/2)!]^2}{\ell!} \qquad \text{for } \ell \text{ even,} \tag{18.5}$$

$$\beta_\ell = \frac{(-1)^{(\ell+1)/2} 2^{\ell-1} \{[(\ell-1)/2]!\}^2}{\ell!} \qquad \text{for } \ell \text{ odd.} \tag{18.6}$$

These normalisation factors are chosen so that the $Q_\ell(x)$ obey the same recurrence relations as the $P_\ell(x)$ (see subsection 18.1.2).

The general solution of Legendre's equation for *integer* ℓ is therefore

$$y(x) = c_1 P_\ell(x) + c_2 Q_\ell(x), \tag{18.7}$$

where $P_\ell(x)$ is a polynomial of order ℓ, and so converges for all x, and $Q_\ell(x)$ is an infinite series that converges only for $|x| < 1$.[§]

By using the Wronskian method, section 16.4, we may obtain closed forms for the $Q_\ell(x)$.

► *Use the Wronskian method to find a closed-form expression for $Q_0(x)$.*

From (16.25) a second solution to Legendre's equation (18.1), with $\ell = 0$, is

$$\begin{aligned} y_2(x) &= P_0(x) \int^x \frac{1}{[P_0(u)]^2} \exp\left(\int^u \frac{2v}{1-v^2}\, dv\right) du \\ &= \int^x \exp\left[-\ln(1-u^2)\right] du \\ &= \int^x \frac{du}{(1-u^2)} = \tfrac{1}{2}\ln\left(\frac{1+x}{1-x}\right), \end{aligned} \tag{18.8}$$

where in the second line we have used the fact that $P_0(x) = 1$.

All that remains is to adjust the normalisation of this solution so that it agrees with (18.5). Expanding the logarithm in (18.8) as a Maclaurin series we obtain

$$y_2(x) = x + \frac{x^3}{3} + \frac{x^5}{5} + \cdots.$$

Comparing this with the expression for $Q_0(x)$, using (18.4) with $\ell = 0$ and the normalisation (18.5), we find that $y_2(x)$ is already correctly normalised, and so

$$Q_0(x) = \tfrac{1}{2}\ln\left(\frac{1+x}{1-x}\right).$$

Of course, we might have recognised the series (18.4) for $\ell = 0$, but to do so for larger ℓ would prove progressively more difficult. ◄

Using the above method for $\ell = 1$, we find

$$Q_1(x) = \tfrac{1}{2}x \ln\left(\frac{1+x}{1-x}\right) - 1.$$

Closed forms for higher-order $Q_\ell(x)$ may now be found using the recurrence relation (18.27) derived in the next subsection. The first few Legendre functions of the second kind are plotted in figure 18.2.

18.1.2 Properties of Legendre polynomials

As stated earlier, when encountered in physical problems the variable x in Legendre's equation is usually the cosine of the polar angle θ in spherical polar coordinates, and we then require the solution $y(x)$ to be regular at $x = \pm 1$, which corresponds to $\theta = 0$ or $\theta = \pi$. For this to occur we require the equation to have a polynomial solution, and so ℓ must be an integer. Furthermore, we also require

[§] It is possible, in fact, to find a second solution in terms of an infinite series of *negative* powers of x that is finite for $|x| > 1$ (see exercise 16.16).

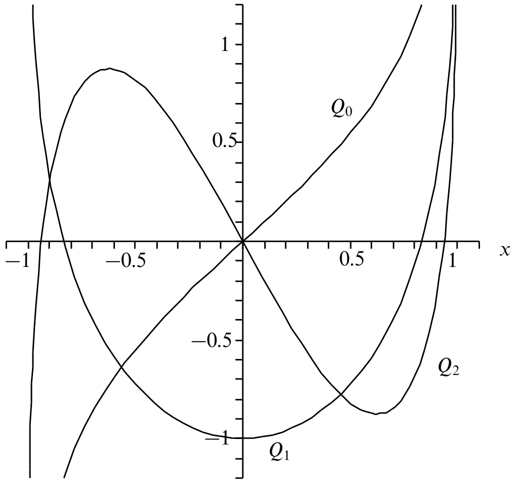

Figure 18.2 The first three Legendre functions of the second kind.

the coefficient c_2 of the function $Q_\ell(x)$ in (18.7) to be zero, since $Q_\ell(x)$ is singular at $x = \pm 1$, with the result that the general solution is simply some multiple of the relevant Legendre polynomial $P_\ell(x)$. In this section we will study the properties of the Legendre polynomials $P_\ell(x)$ in some detail.

Rodrigues' formula

As an aid to establishing further properties of the Legendre polynomials we now develop Rodrigues' representation of these functions. Rodrigues' formula for the $P_\ell(x)$ is

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}(x^2-1)^\ell. \tag{18.9}$$

To prove that this is a representation we let $u = (x^2-1)^\ell$, so that $u' = 2\ell x(x^2-1)^{\ell-1}$ and

$$(x^2-1)u' - 2\ell x u = 0.$$

If we differentiate this expression $\ell + 1$ times using Leibnitz' theorem, we obtain

$$\left[(x^2-1)u^{(\ell+2)} + 2x(\ell+1)u^{(\ell+1)} + \ell(\ell+1)u^{(\ell)}\right] - 2\ell\left[xu^{(\ell+1)} + (\ell+1)u^{(\ell)}\right] = 0,$$

which reduces to

$$(x^2-1)u^{(\ell+2)}+2xu^{(\ell+1)}-\ell(\ell+1)u^{(\ell)}=0.$$

Changing the sign all through, we recover Legendre's equation (18.1) with $u^{(\ell)}$ as the dependent variable. Since, from (18.9), ℓ is an integer and $u^{(\ell)}$ is regular at $x=\pm 1$, we may make the identification

$$u^{(\ell)}(x)=c_\ell P_\ell(x), \tag{18.10}$$

for some constant c_ℓ that depends on ℓ. To establish the value of c_ℓ we note that the only term in the expression for the ℓth derivative of $(x^2-1)^\ell$ that does not contain a factor x^2-1, and therefore does not vanish at $x=1$, is $(2x)^\ell \ell!(x^2-1)^0$. Putting $x=1$ in (18.10) and recalling that $P_\ell(1)=1$, therefore shows that $c_\ell=2^\ell \ell!$, thus completing the proof of Rodrigues' formula (18.9).

►*Use Rodrigues' formula to show that*

$$I_\ell=\int_{-1}^{1}P_\ell(x)P_\ell(x)\,dx=\frac{2}{2\ell+1}. \tag{18.11}$$

The result is trivially obvious for $\ell=0$ and so we assume $\ell\geq 1$. Then, by Rodrigues' formula,

$$I_\ell=\frac{1}{2^{2\ell}(\ell!)^2}\int_{-1}^{1}\left[\frac{d^\ell(x^2-1)^\ell}{dx^\ell}\right]\left[\frac{d^\ell(x^2-1)^\ell}{dx^\ell}\right]dx.$$

Repeated integration by parts, with all boundary terms vanishing, reduces this to

$$\begin{aligned}I_\ell&=\frac{(-1)^\ell}{2^{2\ell}(\ell!)^2}\int_{-1}^{1}(x^2-1)^\ell\frac{d^{2\ell}}{dx^{2\ell}}(x^2-1)^\ell\,dx\\&=\frac{(2\ell)!}{2^{2\ell}(\ell!)^2}\int_{-1}^{1}(1-x^2)^\ell\,dx.\end{aligned}$$

If we write

$$K_\ell=\int_{-1}^{1}(1-x^2)^\ell\,dx,$$

then integration by parts (taking a factor 1 as the second part) gives

$$K_\ell=\int_{-1}^{1}2\ell x^2(1-x^2)^{\ell-1}\,dx.$$

Writing $2\ell x^2$ as $2\ell-2\ell(1-x^2)$ we obtain

$$\begin{aligned}K_\ell&=2\ell\int_{-1}^{1}(1-x^2)^{\ell-1}\,dx-2\ell\int_{-1}^{1}(1-x^2)^\ell\,dx\\&=2\ell K_{\ell-1}-2\ell K_\ell\end{aligned}$$

and hence the recurrence relation $(2\ell+1)K_\ell=2\ell K_{\ell-1}$. We therefore find

$$K_\ell=\frac{2\ell}{2\ell+1}\,\frac{2\ell-2}{2\ell-1}\cdots\frac{2}{3}K_0=2^\ell\ell!\frac{2^\ell\ell!}{(2\ell+1)!}2=\frac{2^{2\ell+1}(\ell!)^2}{(2\ell+1)!},$$

which, when substituted into the expression for I_ℓ, establishes the required result. ◄

Mutual orthogonality

In section 17.4, we noted that Legendre's equation was of Sturm–Liouville form with $p = 1 - x^2$, $q = 0$, $\lambda = \ell(\ell + 1)$ and $\rho = 1$, and that its natural interval was $[-1, 1]$. Since the Legendre polynomials $P_\ell(x)$ are regular at the end-points $x = \pm 1$, they must be mutually orthogonal over this interval, i.e.

$$\int_{-1}^{1} P_\ell(x) P_k(x)\, dx = 0 \qquad \text{if } \ell \neq k. \tag{18.12}$$

Although this result follows from the general considerations of the previous chapter, it may also be proved directly, as shown in the following example.

►*Prove directly that the Legendre polynomials $P_\ell(x)$ are mutually orthogonal over the interval $-1 < x < 1$.*

Since the $P_\ell(x)$ satisfy Legendre's equation we may write

$$\left[(1 - x^2) P_\ell'\right]' + \ell(\ell + 1) P_\ell = 0,$$

where $P_\ell' = dP_\ell/dx$. Multiplying through by P_k and integrating from $x = -1$ to $x = 1$, we obtain

$$\int_{-1}^{1} P_k \left[(1 - x^2) P_\ell'\right]'\, dx + \int_{-1}^{1} P_k \ell(\ell + 1) P_\ell\, dx = 0.$$

Integrating the first term by parts and noting that the boundary contribution vanishes at both limits because of the factor $1 - x^2$, we find

$$-\int_{-1}^{1} P_k' (1 - x^2) P_\ell'\, dx + \int_{-1}^{1} P_k \ell(\ell + 1) P_\ell\, dx = 0.$$

Now, if we reverse the roles of ℓ and k and subtract one expression from the other, we conclude that

$$[k(k + 1) - \ell(\ell + 1)] \int_{-1}^{1} P_k P_\ell\, dx = 0,$$

and therefore, since $k \neq \ell$, we must have the result (18.12). As a particular case, we note that if we put $k = 0$ we obtain

$$\int_{-1}^{1} P_\ell(x)\, dx = 0 \qquad \text{for } \ell \neq 0. \blacktriangleleft$$

As we discussed in the previous chapter, the mutual orthogonality (and completeness) of the $P_\ell(x)$ means that any reasonable function $f(x)$ (i.e. one obeying the Dirichlet conditions discussed at the start of chapter 12) can be expressed in the interval $|x| < 1$ as an infinite sum of Legendre polynomials,

$$f(x) = \sum_{\ell=0}^{\infty} a_\ell P_\ell(x), \tag{18.13}$$

where the coefficients a_ℓ are given by

$$a_\ell = \frac{2\ell + 1}{2} \int_{-1}^{1} f(x) P_\ell(x)\, dx. \tag{18.14}$$

►*Prove the expression (18.14) for the coefficients in the Legendre polynomial expansion of a function $f(x)$.*

If we multiply (18.13) by $P_k(x)$ and integrate from $x = -1$ to $x = 1$ then we obtain

$$\int_{-1}^{1} P_k(x) f(x)\, dx = \sum_{\ell=0}^{\infty} a_\ell \int_{-1}^{1} P_k(x) P_\ell(x)\, dx$$
$$= a_k \int_{-1}^{1} P_k(x) P_k(x)\, dx = \frac{2a_k}{2k+1},$$

where we have used the orthogonality property (18.12) and the normalisation property (18.11). ◄

Generating function

A useful device for manipulating and studying sequences of functions or quantities labelled by an integer variable (here, the Legendre polynomials $P_\ell(x)$ labelled by ℓ) is a *generating function.* The generating function has perhaps its greatest utility in the area of probability theory (see chapter 30). However, it is also a great convenience in our present study.

The generating function for, say, a series of functions $f_n(x)$ for $n = 0, 1, 2, \ldots$ is a function $G(x, h)$ containing, as well as x, a dummy variable h such that

$$G(x, h) = \sum_{n=0}^{\infty} f_n(x) h^n,$$

i.e. $f_n(x)$ is the coefficient of h^n in the expansion of G in powers of h. The utility of the device lies in the fact that sometimes it is possible to find a closed form for $G(x, h)$.

For our study of Legendre polynomials let us consider the functions $P_n(x)$ defined by the equation

$$G(x, h) = (1 - 2xh + h^2)^{-1/2} = \sum_{n=0}^{\infty} P_n(x) h^n. \tag{18.15}$$

As we show below, the functions so defined are identical to the Legendre polynomials and the function $(1 - 2xh + h^2)^{-1/2}$ is in fact the generating function for them. In the process we will also deduce several useful relationships between the various polynomials and their derivatives.

►*Show that the functions $P_n(x)$ defined by (18.15) satisfy Legendre's equation*

In the following $dP_n(x)/dx$ will be denoted by P_n'. Firstly, we differentiate the defining equation (18.15) with respect to x and get

$$h(1 - 2xh + h^2)^{-3/2} = \sum P_n' h^n. \tag{18.16}$$

Also, we differentiate (18.15) with respect to h to yield

$$(x - h)(1 - 2xh + h^2)^{-3/2} = \sum n P_n h^{n-1}. \tag{18.17}$$

Equation (18.16) can then be written, using (18.15), as

$$h\sum P_n h^n = (1 - 2xh + h^2)\sum P_n' h^n,$$

and equating the coefficients of h^{n+1} we obtain the recurrence relation

$$P_n = P_{n+1}' - 2xP_n' + P_{n-1}'. \qquad (18.18)$$

Equations (18.16) and (18.17) can be combined as

$$(x - h)\sum P_n' h^n = h\sum nP_n h^{n-1},$$

from which the coefficent of h^n yields a second recurrence relation,

$$xP_n' - P_{n-1}' = nP_n; \qquad (18.19)$$

eliminating P_{n-1}' between (18.18) and (18.19) then gives the further result

$$(n + 1)P_n = P_{n+1}' - xP_n'. \qquad (18.20)$$

If we now take the result (18.20) with n replaced by $n - 1$ and add x times (18.19) to it we obtain

$$(1 - x^2)P_n' = n(P_{n-1} - xP_n). \qquad (18.21)$$

Finally, differentiating both sides with respect to x and using (18.19) again, we find

$$\begin{aligned}(1 - x^2)P_n'' - 2xP_n' &= n[(P_{n-1}' - xP_n') - P_n]\\ &= n(-nP_n - P_n) = -n(n + 1)P_n,\end{aligned}$$

and so the P_n defined by (18.15) do indeed satisfy Legendre's equation. ◀

The above example shows that the functions $P_n(x)$ defined by (18.15) satisfy Legendre's equation with $\ell = n$ (an integer) and, also from (18.15), these functions are regular at $x = \pm 1$. Thus P_n must be some multiple of the nth Legendre polynomial. It therefore remains only to verify the normalisation. This is easily done at $x = 1$, when G becomes

$$G(1, h) = [(1 - h)^2]^{-1/2} = 1 + h + h^2 + \cdots,$$

and we can see that all the P_n so defined have $P_n(1) = 1$ as required, and are thus identical to the Legendre polynomials.

A particular use of the generating function (18.15) is in representing the inverse distance between two points in three-dimensional space in terms of Legendre polynomials. If two points $\mathbf{r}$ and $\mathbf{r}'$ are at distances r and r', respectively, from the origin, with $r' < r$, then

$$\begin{aligned}\frac{1}{|\mathbf{r} - \mathbf{r}'|} &= \frac{1}{(r^2 + r'^2 - 2rr'\cos\theta)^{1/2}}\\ &= \frac{1}{r[1 - 2(r'/r)\cos\theta + (r'/r)^2]^{1/2}}\\ &= \frac{1}{r}\sum_{\ell=0}^{\infty}\left(\frac{r'}{r}\right)^{\ell} P_\ell(\cos\theta), \qquad (18.22)\end{aligned}$$

where θ is the angle between the two position vectors $\mathbf{r}$ and $\mathbf{r}'$. If $r' > r$, however,

r and r' must be exchanged in (18.22) or the series would not converge. This result may be used, for example, to write down the electrostatic potential at a point $\mathbf{r}$ due to a charge q at the point $\mathbf{r}'$. Thus, in the case $r' < r$, this is given by

$$V(\mathbf{r}) = \frac{q}{4\pi\epsilon_0 r}\sum_{\ell=0}^{\infty}\left(\frac{r'}{r}\right)^{\ell} P_\ell(\cos\theta).$$

We note that in the special case where the charge is at the origin, and $r' = 0$, only the $\ell = 0$ term in the series is non-zero and the expression reduces correctly to the familiar form $V(\mathbf{r}) = q/(4\pi\epsilon_0 r)$.

Recurrence relations

In our discussion of the generating function above, we derived several useful recurrence relations satisfied by the Legendre polynomials $P_n(x)$. In particular, from (18.18), we have the four-term recurrence relation

$$P'_{n+1} + P'_{n-1} = P_n + 2xP'_n.$$

Also, from (18.19)–(18.21), we have the three-term recurrence relations

$$P'_{n+1} = (n+1)P_n + xP'_n, \tag{18.23}$$
$$P'_{n-1} = -nP_n + xP'_n, \tag{18.24}$$
$$(1-x^2)P'_n = n(P_{n-1} - xP_n), \tag{18.25}$$
$$(2n+1)P_n = P'_{n+1} - P'_{n-1}, \tag{18.26}$$

where the final relation is obtained immediately by subtracting the second from the first. Many other useful recurrence relations can be derived from those given above and from the generating function.

►*Prove the recurrence relation*

$$(n+1)P_{n+1} = (2n+1)xP_n - nP_{n-1}. \tag{18.27}$$

Substituting from (18.15) into (18.17), we find

$$(x-h)\sum P_n h^n = (1 - 2xh + h^2)\sum nP_n h^{n-1}.$$

Equating coefficients of h^n we obtain

$$xP_n - P_{n-1} = (n+1)P_{n+1} - 2xnP_n + (n-1)P_{n-1},$$

which on rearrangement gives the stated result. ◄

The recurrence relation derived in the above example is particularly useful in evaluating $P_n(x)$ for a given value of x. One starts with $P_0(x) = 1$ and $P_1(x) = x$ and iterates the recurrence relation until $P_n(x)$ is obtained.

18.2 Associated Legendre functions

The associated Legendre equation has the form

$$(1-x^2)y'' - 2xy' + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right] y = 0, \tag{18.28}$$

which has three regular singular points at $x = -1, 1, \infty$ and reduces to Legendre's equation (18.1) when $m = 0$. It occurs in physical applications involving the operator ∇^2, when expressed in spherical polars. In such cases, $-\ell \leq m \leq \ell$ and m is restricted to integer values, which we will assume from here on. As was the case for Legendre's equation, in normal usage the variable x is the cosine of the polar angle in spherical polars, and thus $-1 \leq x \leq 1$. Any solution of (18.28) is called an *associated Legendre function.*

The point $x = 0$ is an ordinary point of (18.28), and one could obtain series solutions of the form $y = \sum_{n=0} a_n x^n$ in the same manner as that used for Legendre's equation. In this case, however, it is more instructive to note that if $u(x)$ is a solution of Legendre's equation (18.1), then

$$y(x) = (1-x^2)^{|m|/2} \frac{d^{|m|}u}{dx^{|m|}} \tag{18.29}$$

is a solution of the associated equation (18.28).

►*Prove that if $u(x)$ is a solution of Legendre's equation, then $y(x)$ given in (18.29) is a solution of the associated equation.*

For simplicity, let us begin by assuming that m is non-negative. Legendre's equation for u reads

$$(1-x^2)u'' - 2xu' + \ell(\ell+1)u = 0,$$

and, on differentiating this equation m times using Leibnitz' theorem, we obtain

$$(1-x^2)v'' - 2x(m+1)v' + (\ell-m)(\ell+m+1)v = 0, \tag{18.30}$$

where $v(x) = d^m u/dx^m$. On setting

$$y(x) = (1-x^2)^{m/2} v(x),$$

the derivatives v' and v'' may be written as

$$v' = (1-x^2)^{-m/2}\left(y' + \frac{mx}{1-x^2}y\right),$$

$$v'' = (1-x^2)^{-m/2}\left[y'' + \frac{2mx}{1-x^2}y' + \frac{m}{1-x^2}y + \frac{m(m+2)x^2}{(1-x^2)^2}y\right].$$

Substituting these expressions into (18.30) and simplifying, we obtain

$$(1-x^2)y'' - 2xy' + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right] y = 0,$$

which shows that y is a solution of the associated Legendre equation (18.28). Finally, we note that if m is negative, the value of m^2 is unchanged, and so a solution for positive m is also a solution for the corresponding negative value of m. ◄

From the two linearly independent series solutions to Legendre's equation given in (18.3) and (18.4), which we now denote by $u_1(x)$ and $u_2(x)$, we may obtain two linearly-independent series solutions, $y_1(x)$ and $y_2(x)$, to the associated equation by using (18.29). From the general discussion of the convergence of power series given in section 4.5.1, we see that both $y_1(x)$ and $y_2(x)$ will also converge for $|x| < 1$. Hence the general solution to (18.28) in this range is given by

$$y(x) = c_1 y_1(x) + c_2 y_2(x).$$

18.2.1 Associated Legendre functions for integer ℓ

If ℓ and m are both integers, as is the case in many physical applications, then the general solution to (18.28) is denoted by

$$y(x) = c_1 P_\ell^m(x) + c_2 Q_\ell^m(x), \tag{18.31}$$

where $P_\ell^m(x)$ and $Q_\ell^m(x)$ are associated Legendre functions of the first and second kind, respectively. For non-negative values of m, these functions are related to the ordinary Legendre functions for integer ℓ by

$$P_\ell^m(x) = (1-x^2)^{m/2}\frac{d^m P_\ell}{dx^m}, \qquad Q_\ell^m(x) = (1-x^2)^{m/2}\frac{d^m Q_\ell}{dx^m}. \tag{18.32}$$

We see immediately that, as required, the associated Legendre functions reduce to the ordinary Legendre functions when $m = 0$. Since it is m^2 that appears in the associated Legendre equation (18.28), the associated Legendre functions for negative m values must be proportional to the corresponding function for non-negative m. The constant of proportionality is a matter of convention. For the $P_\ell^m(x)$ it is usual to regard the definition (18.32) as being valid also for negative m values. Although differentiating a negative number of times is not defined, when $P_\ell(x)$ is expressed in terms of the Rodrigues' formula (18.9), this problem does not occur for $-\ell \le m \le \ell$.[§] In this case,

$$P_\ell^{-m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(x). \tag{18.33}$$

►*Prove the result (18.33).*

From (18.32) and the Rodrigues' formula (18.9) for the Legendre polynomials, we have

$$P_\ell^m(x) = \frac{1}{2^\ell \ell!}(1-x^2)^{m/2}\frac{d^{\ell+m}}{dx^{\ell+m}}(x^2-1)^\ell,$$

and, without loss of generality, we may assume that m is non-negative. It is convenient to

[§] Some authors define $P_\ell^{-m}(x) = P_\ell^m(x)$, and similarly for the $Q_\ell^m(x)$, in which case m is replaced by $|m|$ in the definitions (18.32). It should be noted that, in this case, many of the results presented in this section also require m to be replaced by $|m|$.

write $(x^2-1)=(x+1)(x-1)$ and use Leibnitz' theorem to evaluate the derivative, which yields

$$P_\ell^m(x)=\frac{1}{2^\ell \ell!}(1-x^2)^{m/2}\sum_{r=0}^{\ell+m}\frac{(\ell+m)!}{r!(\ell+m-r)!}\frac{d^r(x+1)^\ell}{dx^r}\frac{d^{\ell+m-r}(x-1)^\ell}{dx^{\ell+m-r}}.$$

Considering the two derivative factors in a term in the summation, we note that the first is non-zero only for $r\le\ell$ and the second is non-zero for $\ell+m-r\le\ell$. Combining these conditions yields $m\le r\le\ell$. Performing the derivatives, we thus obtain

$$\begin{aligned}P_\ell^m(x)&=\frac{1}{2^\ell \ell!}(1-x^2)^{m/2}\sum_{r=m}^{\ell}\frac{(\ell+m)!}{r!(\ell+m-r)!}\frac{\ell!(x+1)^{\ell-r}}{(\ell-r)!}\frac{\ell!(x-1)^{r-m}}{(r-m)!}\\&=(-1)^{m/2}\frac{\ell!(\ell+m)!}{2^\ell}\sum_{r=m}^{\ell}\frac{(x+1)^{\ell-r+\frac{m}{2}}(x-1)^{r-\frac{m}{2}}}{r!(\ell+m-r)!(\ell-r)!(r-m)!}.\end{aligned}\qquad(18.34)$$

Repeating the above calculation for $P_\ell^{-m}(x)$ and identifying once more those terms in the sum that are non-zero, we find

$$\begin{aligned}P_\ell^{-m}(x)&=(-1)^{-m/2}\frac{\ell!(\ell-m)!}{2^\ell}\sum_{r=0}^{\ell-m}\frac{(x+1)^{\ell-r-\frac{m}{2}}(x-1)^{r+\frac{m}{2}}}{r!(\ell-m-r)!(\ell-r)!(r+m)!}\\&=(-1)^{-m/2}\frac{\ell!(\ell-m)!}{2^\ell}\sum_{\bar r=m}^{\ell}\frac{(x+1)^{\ell-\bar r+\frac{m}{2}}(x-1)^{\bar r-\frac{m}{2}}}{(\bar r-m)!(\ell-\bar r)!(\ell+m-\bar r)!\bar r!},\end{aligned}\qquad(18.35)$$

where, in the second equality, we have rewritten the summation in terms of the new index $\bar r=r+m$. Comparing (18.34) and (18.35), we immediately arrive at the required result (18.33). ◀

Since $P_\ell(x)$ is a polynomial of order ℓ, we have $P_\ell^m(x)=0$ for $|m|>\ell$. From its definition, it is clear that $P_\ell^m(x)$ is also a polynomial of order ℓ if m is even, but contains the factor $(1-x^2)$ to a fractional power if m is odd. In either case, $P_\ell^m(x)$ is regular at $x=\pm1$. The first few associated Legendre functions of the first kind are easily constructed and are given by (omitting the $m=0$ cases)

$$\begin{aligned}P_1^1(x)&=(1-x^2)^{1/2}, & P_2^1(x)&=3x(1-x^2)^{1/2},\\P_2^2(x)&=3(1-x^2), & P_3^1(x)&=\tfrac{3}{2}(5x^2-1)(1-x^2)^{1/2},\\P_3^2(x)&=15x(1-x^2), & P_3^3(x)&=15(1-x^2)^{3/2}.\end{aligned}$$

Finally, we note that the associated Legendre functions of the second kind $Q_\ell^m(x)$, like $Q_\ell(x)$, are singular at $x=\pm1$.

18.2.2 Properties of associated Legendre functions $P_\ell^m(x)$

When encountered in physical problems, the variable x in the associated Legendre equation (as in the ordinary Legendre equation) is usually the cosine of the polar angle θ in spherical polar coordinates, and we then require the solution $y(x)$ to be regular at $x=\pm1$ (corresponding to $\theta=0$ or $\theta=\pi$). For this to occur, we require ℓ to be an integer and the coefficient c_2 of the function $Q_\ell^m(x)$ in (18.31) to be zero, since $Q_\ell^m(x)$ is singular at $x = \pm 1$, with the result that the general solution is simply some multiple of one of the associated Legendre functions of the first kind, $P_\ell^m(x)$. We will study the further properties of these functions in the remainder of this subsection.

Mutual orthogonality

As noted in section 17.4, the associated Legendre equation is of Sturm–Liouville form $(py)' + qy + \lambda\rho y = 0$, with $p = 1 - x^2$, $q = -m^2/(1 - x^2)$, $\lambda = \ell(\ell + 1)$ and $\rho = 1$, and its natural interval is thus $[-1, 1]$. Since the associated Legendre functions $P_\ell^m(x)$ are regular at the end-points $x = \pm 1$, they must be mutually orthogonal over this interval for a fixed value of m, i.e.

$$\int_{-1}^{1} P_\ell^m(x) P_k^m(x)\, dx = 0 \qquad \text{if } \ell \neq k. \tag{18.36}$$

This result may also be proved directly in a manner similar to that used for demonstrating the orthogonality of the Legendre polynomials $P_\ell(x)$ in section 18.1.2. Note that the value of m must be the same for the two associated Legendre functions for (18.36) to hold. The normalisation condition when $\ell = k$ may be obtained using the Rodrigues' formula, as shown in the following example.

►*Show that*

$$I_{\ell m} \equiv \int_{-1}^{1} P_\ell^m(x) P_\ell^m(x)\, dx = \frac{2}{2\ell + 1} \frac{(\ell + m)!}{(\ell - m)!}. \tag{18.37}$$

From the definition (18.32) and the Rodrigues' formula (18.9) for $P_\ell(x)$, we may write

$$I_{\ell m} = \frac{1}{2^{2\ell}(\ell!)^2} \int_{-1}^{1} \left[(1 - x^2)^m \frac{d^{\ell+m}(x^2 - 1)^\ell}{dx^{\ell+m}} \right] \left[\frac{d^{\ell+m}(x^2 - 1)^\ell}{dx^{\ell+m}} \right] dx,$$

where the square brackets identify the factors to be used when integrating by parts. Performing the integration by parts $\ell + m$ times, and noting that all boundary terms vanish, we obtain

$$I_{\ell m} = \frac{(-1)^{\ell+m}}{2^{2\ell}(\ell!)^2} \int_{-1}^{1} (x^2 - 1)^\ell \frac{d^{\ell+m}}{dx^{\ell+m}} \left[(1 - x^2)^m \frac{d^{\ell+m}(x^2 - 1)^\ell}{dx^{\ell+m}} \right] dx.$$

Using Leibnitz' theorem, the second factor in the integrand may be written as

$$\frac{d^{\ell+m}}{dx^{\ell+m}} \left[(1 - x^2)^m \frac{d^{\ell+m}(x^2 - 1)^\ell}{dx^{\ell+m}} \right] = \sum_{r=0}^{\ell+m} \frac{(\ell + m)!}{r!(\ell + m - r)!} \frac{d^r(1 - x^2)^m}{dx^r} \frac{d^{2\ell+2m-r}(x^2 - 1)^\ell}{dx^{2\ell+2m-r}}.$$

Considering the two derivative factors in a term in the summation on the RHS, we see that the first is non-zero only for $r \leq 2m$, whereas the second is non-zero only for $2\ell + 2m - r \leq 2\ell$. Combining these conditions, we find that the only non-zero term in the sum is that for which $r = 2m$. Thus, we may write

$$I_{\ell m} = \frac{(-1)^{\ell+m}}{2^{2\ell}(\ell!)^2} \frac{(\ell + m)!}{(2m)!(\ell - m)!} \int_{-1}^{1} (1 - x^2)^\ell \frac{d^{2m}(1 - x^2)^m}{dx^{2m}} \frac{d^{2\ell}(1 - x^2)^\ell}{dx^{2\ell}}\, dx.$$

Since $d^{2\ell}(1-x^2)^\ell/dx^{2\ell} = (-1)^\ell(2\ell)!$, and noting that $(-1)^{2\ell+2m} = 1$, we have

$$I_{\ell m} = \frac{1}{2^{2\ell}(\ell!)^2}\frac{(2\ell)!(\ell+m)!}{(\ell-m)!}\int_{-1}^{1}(1-x^2)^\ell\,dx.$$

We have already shown in section 18.1.2 that

$$K_\ell \equiv \int_{-1}^{1}(1-x^2)^\ell\,dx = \frac{2^{2\ell+1}(\ell!)^2}{(2\ell+1)!},$$

and so we obtain the final result

$$I_{\ell m} = \frac{2}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}. \blacktriangleleft$$

The orthogonality and normalisation conditions, (18.36) and (18.37) respectively, mean that the associated Legendre functions $P_\ell^m(x)$, with m fixed, may be used in a similar way to the Legendre polynomials to expand any reasonable function $f(x)$ on the interval $|x| < 1$ in a series of the form

$$f(x) = \sum_{k=0}^{\infty} a_{m+k}P_{m+k}^m(x), \tag{18.38}$$

where, in this case, the coefficients are given by

$$a_\ell = \frac{2\ell+1}{2}\frac{(\ell-m)!}{(\ell+m)!}\int_{-1}^{1} f(x)P_\ell^m(x)\,dx.$$

We note that the series takes the form (18.38) because $P_\ell^m(x) = 0$ for $m > \ell$.

Finally, it is worth noting that the associated Legendre functions $P_\ell^m(x)$ must also obey a second orthogonality relationship. This has to be so because one may equally well write the associated Legendre equation (18.28) in Sturm–Liouville form $(py)'+qy+\lambda\rho y = 0$, with $p = 1-x^2$, $q = \ell(\ell+1)$, $\lambda = -m^2$ and $\rho = (1-x^2)^{-1}$; once again the natural interval is $[-1, 1]$. Since the associated Legendre functions $P_\ell^m(x)$ are regular at the end-points $x = \pm 1$, they must therefore be mutually orthogonal with respect to the weight function $(1-x^2)^{-1}$ over this interval for a fixed value of ℓ, i.e.

$$\int_{-1}^{1} P_\ell^m(x)P_\ell^k(x)(1-x^2)^{-1}\,dx = 0 \qquad \text{if } |m| \neq |k|. \tag{18.39}$$

One may also show straightforwardly that the corresponding normalisation condition when $m = k$ is given by

$$\int_{-1}^{1} P_\ell^m(x)P_\ell^m(x)(1-x^2)^{-1}\,dx = \frac{(\ell+m)!}{m(\ell-m)!}.$$

In solving physical problems, however, the orthogonality condition (18.39) is not of any practical use.

Generating function

The generating function for associated Legendre functions can be easily derived by combining their definition (18.32) with the generating function for the Legendre polynomials given in (18.15). We find that

$$G(x,h) = \frac{(2m)!(1-x^2)^{m/2}}{2^m m!(1-2hx+h^2)^{m+1/2}} = \sum_{n=0}^{\infty} P_{n+m}^m(x)h^n. \tag{18.40}$$

►*Derive the expression (18.40) for the associated Legendre generating function.*

The generating function (18.15) for the Legendre polynomials reads

$$\sum_{n=0}^{\infty} P_n h^n = (1-2xh+h^2)^{-1/2}.$$

Differentiating both sides of this result m times (assumimg m to be non-negative), mutliplying through by $(1-x^2)^{m/2}$ and using the definition (18.32) of the associated Legendre functions, we obtain

$$\sum_{n=0}^{\infty} P_n^m h^n = (1-x^2)^{m/2}\frac{d^m}{dx^m}(1-2xh+h^2)^{-1/2}.$$

Performing the derivatives on the RHS gives

$$\sum_{n=0}^{\infty} P_n^m h^n = \frac{1\cdot 3\cdot 5\cdots(2m-1)(1-x^2)^{m/2}h^m}{(1-2xh+h^2)^{m+1/2}}.$$

Dividing through by h^m, re-indexing the summation on the LHS and noting that, quite generally,

$$1\cdot 3\cdot 5\cdots(2r-1) = \frac{1\cdot 2\cdot 3\cdots 2r}{2\cdot 4\cdot 6\cdots 2r} = \frac{(2r)!}{2^r r!},$$

we obtain the final result (18.40). ◄

Recurrence relations

As one might expect, the associated Legendre functions satisfy certain recurrence relations. Indeed, the presence of the two indices n and m means that a much wider range of recurrence relations may be derived. Here we shall content ourselves with quoting just four of the most useful relations:

$$P_n^{m+1} = \frac{2mx}{(1-x^2)^{1/2}}P_n^m + [m(m-1)-n(n+1)]P_n^{m-1}, \tag{18.41}$$

$$(2n+1)xP_n^m = (n+m)P_{n-1}^m + (n-m+1)P_{n+1}^m, \tag{18.42}$$

$$(2n+1)(1-x^2)^{1/2}P_n^m = P_{n+1}^{m+1} - P_{n-1}^{m+1}, \tag{18.43}$$

$$2(1-x^2)^{1/2}(P_n^m)' = P_n^{m+1} - (n+m)(n-m+1)P_n^{m-1}. \tag{18.44}$$

We note that, by virtue of our adopted definition (18.32), these recurrence relations are equally valid for negative and non-negative values of m. These relations may be derived in a number of ways, such as using the generating function (18.40) or by differentiation of the recurrence relations for the Legendre polynomials $P_\ell(x)$.

►*Use the recurrence relation* $(2n+1)P_n = P'_{n+1} - P'_{n-1}$ *for Legendre polynomials to derive the result (18.43).*

Differentiating the recurrence relation for the Legendre polynomials m times, we have

$$(2n+1)\frac{d^m P_n}{dx^m} = \frac{d^{m+1} P_{n+1}}{dx^{m+1}} - \frac{d^{m+1} P_{n-1}}{dx^{m+1}}.$$

Multiplying through by $(1-x^2)^{(m+1)/2}$ and using the definition (18.32) immediately gives the result (18.43). ◄

18.3 Spherical harmonics

The associated Legendre functions discussed in the previous section occur most commonly when obtaining solutions in spherical polar coordinates of Laplace's equation $\nabla^2 u = 0$ (see section 21.3.1). In particular, one finds that, for solutions that are finite on the polar axis, the angular part of the solution is given by

$$\Theta(\theta)\Phi(\phi) = P_\ell^m(\cos\theta)(C\cos m\phi + D\sin m\phi),$$

where ℓ and m are integers with $-\ell \le m \le \ell$. This general form is sufficiently common that particular functions of θ and ϕ called *spherical harmonics* are defined and tabulated. The spherical harmonics $Y_\ell^m(\theta,\phi)$ are defined by

$$Y_\ell^m(\theta,\phi) = (-1)^m \left[\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}\right]^{1/2} P_\ell^m(\cos\theta)\exp(im\phi). \tag{18.45}$$

Using (18.33), we note that

$$Y_\ell^{-m}(\theta,\phi) = (-1)^m \left[Y_\ell^m(\theta,\phi)\right]^*,$$

where the asterisk denotes complex conjugation. The first few spherical harmonics $Y_\ell^m(\theta,\phi) \equiv Y_\ell^m$ are as follows:

$$\begin{aligned}
Y_0^0 &= \sqrt{\tfrac{1}{4\pi}}, & Y_1^0 &= \sqrt{\tfrac{3}{4\pi}}\cos\theta,\\
Y_1^{\pm1} &= \mp\sqrt{\tfrac{3}{8\pi}}\sin\theta\exp(\pm i\phi), & Y_2^0 &= \sqrt{\tfrac{5}{16\pi}}(3\cos^2\theta-1),\\
Y_2^{\pm1} &= \mp\sqrt{\tfrac{15}{8\pi}}\sin\theta\cos\theta\exp(\pm i\phi), & Y_2^{\pm2} &= \sqrt{\tfrac{15}{32\pi}}\sin^2\theta\exp(\pm 2i\phi).
\end{aligned}$$

Since they contain as their θ-dependent part the solution P_ℓ^m to the associated Legendre equation, the Y_ℓ^m are mutually orthogonal when integrated from -1 to $+1$ over $d(\cos\theta)$. Their mutual orthogonality with respect to ϕ $(0 \le \phi \le 2\pi)$ is even more obvious. The numerical factor in (18.45) is chosen to make the Y_ℓ^m an orthonormal set, i.e.

$$\int_{-1}^{1}\int_{0}^{2\pi} \left[Y_\ell^m(\theta,\phi)\right]^* Y_{\ell'}^{m'}(\theta,\phi)\, d\phi\, d(\cos\theta) = \delta_{\ell\ell'}\delta_{mm'}. \qquad (18.46)$$

In addition, the spherical harmonics form a complete set in that any reasonable function (i.e. one that is likely to be met in a physical situation) of θ and ϕ can be expanded as a sum of such functions,

$$f(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} a_{\ell m} Y_\ell^m(\theta,\phi), \qquad (18.47)$$

the constants $a_{\ell m}$ being given by

$$a_{\ell m} = \int_{-1}^{1}\int_{0}^{2\pi} \left[Y_\ell^m(\theta,\phi)\right]^* f(\theta,\phi)\, d\phi\, d(\cos\theta). \qquad (18.48)$$

This is in exact analogy with a Fourier series and is a particular example of the general property of Sturm–Liouville solutions.

Aside from the orthonormality condition (18.46), the most important relationship obeyed by the Y_ℓ^m is the *spherical harmonic addition theorem.* This reads

$$P_\ell(\cos\gamma) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi)[Y_\ell^m(\theta',\phi')]^*, \qquad (18.49)$$

where (θ,ϕ) and (θ',ϕ') denote two different directions in our spherical polar coordinate system that are separated by an angle γ. In general, spherical trigonometry (or vector methods) shows that these angles obey the identity

$$\cos\gamma = \cos\theta\,\cos\theta' + \sin\theta\,\sin\theta'\,\cos(\phi-\phi'). \qquad (18.50)$$

►*Prove the spherical harmonic addition theorem (18.49).*

For the sake of brevity, it will be useful to denote the directions (θ,ϕ) and (θ',ϕ') by Ω and Ω', respectively. We will also denote the element of solid angle on the sphere by $d\Omega = d\phi\, d(\cos\theta)$. We begin by deriving the form of the closure relationship obeyed by the spherical harmonics. Using (18.47) and (18.48), and reversing the order of the summation and integration, we may write

$$f(\Omega) = \int_{4\pi} d\Omega'\, f(\Omega')\sum_{\ell m} Y_\ell^{m*}(\Omega')Y_\ell^m(\Omega),$$

where $\sum_{\ell m}$ is a convenient shorthand for the double summation in (18.47). Thus we may write the closure relationship for the spherical harmonics as

$$\sum_{\ell m} Y_\ell^m(\Omega)Y_\ell^{m*}(\Omega') = \delta(\Omega-\Omega'), \qquad (18.51)$$

where $\delta(\Omega-\Omega')$ is a Dirac delta function with the properties that $\delta(\Omega-\Omega')=0$ if $\Omega\neq\Omega'$ and $\int_{4\pi}\delta(\Omega)\, d\Omega = 1$.

Since $\delta(\Omega - \Omega')$ can depend only on the angle γ between the two directions Ω and Ω', we may also expand it in terms of a series of Legendre polynomials of the form

$$\delta(\Omega - \Omega') = \sum_{\ell} b_\ell P_\ell(\cos\gamma). \tag{18.52}$$

From (18.14), the coefficients in this expansion are given by

$$\begin{aligned} b_\ell &= \frac{2\ell+1}{2}\int_{-1}^{1} \delta(\Omega - \Omega')P_\ell(\cos\gamma)\,d(\cos\gamma) \\ &= \frac{2\ell+1}{4\pi}\int_{0}^{2\pi}\int_{-1}^{1} \delta(\Omega - \Omega')P_\ell(\cos\gamma)\,d(\cos\gamma)\,d\psi, \end{aligned}$$

where, in the second equality, we have introduced an additional integration over an azimuthal angle ψ about the direction Ω' (and γ is now the polar angle measured from Ω' to Ω). Since the rest of the integrand does not depend upon ψ, this is equivalent to multiplying it by $2\pi/2\pi$. However, the resulting double integral now has the form of a solid-angle integration over the whole sphere. Moreover, when $\Omega = \Omega'$, the angle γ separating the two directions is zero, and so $\cos\gamma = 1$. Thus, we find

$$b_\ell = \frac{2\ell+1}{4\pi}P_\ell(1) = \frac{2\ell+1}{4\pi},$$

and combining this expression with (18.51) and (18.52) gives

$$\sum_{\ell m} Y_\ell^m(\Omega)Y_\ell^{m*}(\Omega') = \sum_{\ell} \frac{2\ell+1}{4\pi}P_\ell(\cos\gamma). \tag{18.53}$$

Comparing this result with (18.49), we see that, to complete the proof of the addition theorem, we now only need to show that the summations in ℓ on either side of (18.53) can be equated *term by term*.

That such a procedure is valid may be shown by considering an arbitrary rigid rotation of the coordinate axes, thereby defining new spherical polar coordinates $\bar{\Omega}$ on the sphere. Any given spherical harmonic $Y_\ell^m(\bar{\Omega})$ in the new coordinates can be written as a linear combination of the spherical harmonics $Y_\ell^m(\Omega)$ of the old coordinates, *all* having the *same* value of ℓ. Thus,

$$Y_\ell^m(\bar{\Omega}) = \sum_{m'=-\ell}^{\ell} D_\ell^{mm'}Y_\ell^{m'}(\Omega),$$

where the coefficients $D_\ell^{mm'}$ depend on the rotation; note that in this expression Ω and $\bar{\Omega}$ refer to the same direction, but expressed in the two different coordinate systems. If we choose the polar axis of the new coordinate system to lie along the Ω' direction, then from (18.45), with m in that equation set equal to zero, we may write

$$P_\ell(\cos\gamma) = \sqrt{\frac{4\pi}{2\ell+1}}\,Y_\ell^0(\bar{\Omega}) = \sum_{m'=-\ell}^{\ell} C_\ell^{0m'}Y_\ell^{m'}(\Omega)$$

for some set of coefficients C_ℓ^{0m} that depend on Ω'. Thus, we see that the equality (18.53) does indeed hold term by term in ℓ, thus proving the addition theorem (18.49). ◄

18.4 Chebyshev functions

Chebyshev's equation has the form

$$(1 - x^2)y'' - xy' + \nu^2 y = 0, \tag{18.54}$$

and has three regular singular points, at $x = -1, 1, \infty$. By comparing it with (18.1), we see that the Chebyshev equation is very similar in form to Legendre's equation. Despite this similarity, equation (18.54) does not occur very often in physical problems, though its solutions are of considerable importance in numerical analysis. The parameter ν is a given real number, but in nearly all practical applications it takes an integer value. From here on we thus assume that $\nu = n$, where n is a non-negative integer. As was the case for Legendre's equation, in normal usage the variable x is the cosine of an angle, and so $-1 \le x \le 1$. Any solution of (18.54) is called a *Chebyshev function.*

The point $x = 0$ is an ordinary point of (18.54), and so we expect to find two linearly independent solutions of the form $y = \sum_{m=0}^{\infty} a_m x^m$. One could find the recurrence relations for the coefficients a_m in a similar manner to that used for Legendre's equation in section 18.1 (see exercise 16.15). For Chebyshev's equation, however, it is easier and more illuminating to take a different approach. In particular, we note that, on making the substitution $x = \cos\theta$, and consequently $d/dx = (-1/\sin\theta)\, d/d\theta$, Chebyshev's equation becomes (with $\nu = n$)

$$\frac{d^2 y}{d\theta^2} + n^2 y = 0,$$

which is the simple harmonic equation with solutions $\cos n\theta$ and $\sin n\theta$. The corresponding linearly independent solutions of Chebyshev's equation are thus given by

$$T_n(x) = \cos(n \cos^{-1} x) \quad \text{and} \quad V_n(x) = \sin(n \cos^{-1} x). \tag{18.55}$$

It is straightforward to show that the $T_n(x)$ are *polynomials* of order n, whereas the $V_n(x)$ are *not* polynomials

►*Find explicit forms for the series expansions of $T_n(x)$ and $V_n(x)$.*

Writing $x = \cos\theta$, it is convenient first to form the complex superposition

$$\begin{aligned} T_n(x) + iV_n(x) &= \cos n\theta + i \sin n\theta \\ &= (\cos\theta + i\sin\theta)^n \\ &= \left(x + i\sqrt{1-x^2}\right)^n \qquad \text{for } |x| \le 1. \end{aligned}$$

Then, on expanding out the last expression using the binomial theorem, we obtain

$$T_n(x) = x^n - {}^nC_2 x^{n-2}(1-x^2) + {}^nC_4 x^{n-4}(1-x^2)^2 - \cdots, \tag{18.56}$$

$$V_n(x) = \sqrt{1-x^2}\left[{}^nC_1 x^{n-1} - {}^nC_3 x^{n-3}(1-x^2) + {}^nC_5 x^{n-5}(1-x^2)^2 - \cdots\right], \tag{18.57}$$

where ${}^nC_r = n!/[r!(n-r)!]$ is a binomial coefficient. We thus see that $T_n(x)$ is a polynomial of order n, but $V_n(x)$ is not a polynomial. ◄

It is conventional to define the additional functions

$$W_n(x) = (1-x^2)^{-1/2}\, T_{n+1}(x) \quad \text{and} \quad U_n(x) = (1-x^2)^{-1/2}\, V_{n+1}(x). \tag{18.58}$$

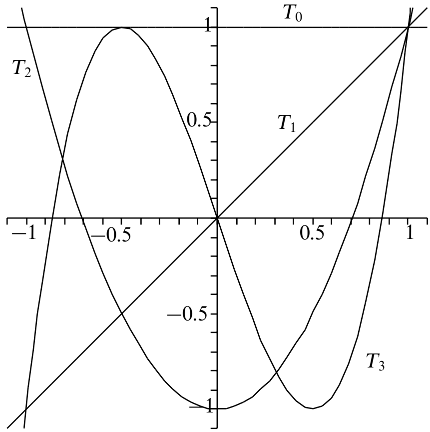

Figure 18.3 The first four Chebyshev polynomials of the first kind.

From (18.56) and (18.57), we see immediately that $U_n(x)$ is a *polynomial* of order n, but that $W_n(x)$ is *not* a polynomial. In practice, it is usual to work entirely in terms of $T_n(x)$ and $U_n(x)$, which are known, respectively, as *Chebyshev polynomials of the first and second kind*. In particular, we note that the general solution to Chebyshev's equation can be written in terms of these polynomials as

$$y(x) = \begin{cases} c_1 T_n(x) + c_2\sqrt{1-x^2}\,U_{n-1}(x) & \text{for } n = 1, 2, 3, \ldots, \\ c_1 + c_2 \sin^{-1} x & \text{for } n = 0. \end{cases}$$

The $n = 0$ solution could also be written as $d_1 + c_2 \cos^{-1} x$ with $d_1 = c_1 + \frac{1}{2}\pi c_2$.

The first few Chebyshev polynomials of the first kind are easily constructed and are given by

$$\begin{aligned} T_0(x) &= 1, & T_1(x) &= x, \\ T_2(x) &= 2x^2 - 1, & T_3(x) &= 4x^3 - 3x, \\ T_4(x) &= 8x^4 - 8x^2 + 1, & T_5(x) &= 16x^5 - 20x^3 + 5x. \end{aligned}$$

The functions $T_0(x)$, $T_1(x)$, $T_2(x)$ and $T_3(x)$ are plotted in figure 18.3. In general, the Chebyshev polynomials $T_n(x)$ satisfy $T_n(-x) = (-1)^n T_n(x)$, which is easily deduced from (18.56). Similarly, it is straightforward to deduce the following

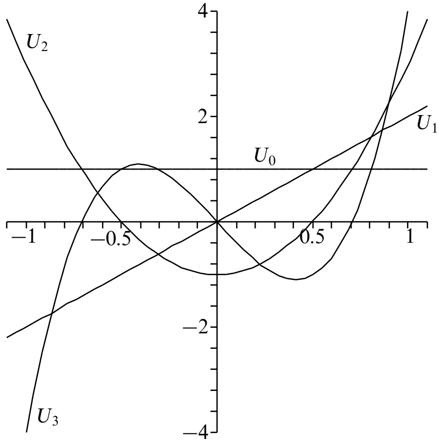

Figure 18.4 The first four Chebyshev polynomials of the second kind.

special values:

$$T_n(1) = 1, \qquad T_n(-1) = (-1)^n, \qquad T_{2n}(0) = (-1)^n, \qquad T_{2n+1}(0) = 0.$$

The first few Chebyshev polynomials of the second kind are also easily found and read

$$\begin{aligned} U_0(x) &= 1, & U_1(x) &= 2x, \\ U_2(x) &= 4x^2 - 1, & U_3(x) &= 8x^3 - 4x, \\ U_4(x) &= 16x^4 - 12x^2 + 1, & U_5(x) &= 32x^5 - 32x^3 + 6x. \end{aligned}$$

The functions $U_0(x)$, $U_1(x)$, $U_2(x)$ and $U_3(x)$ are plotted in figure 18.4. The Chebyshev polynomials $U_n(x)$ also satisfy $U_n(-x) = (-1)^n U_n(x)$, which may be deduced from (18.57) and (18.58), and have the special values:

$$U_n(1) = n + 1, \qquad U_n(-1) = (-1)^n(n + 1), \qquad U_{2n}(0) = (-1)^n, \qquad U_{2n+1}(0) = 0.$$

►*Show that the Chebyshev polynomials $U_n(x)$ satisfy the differential equation*

$$(1 - x^2)U_n''(x) - 3xU_n'(x) + n(n + 2)U_n(x) = 0. \tag{18.59}$$

From (18.58), we have $V_{n+1} = (1 - x^2)^{1/2}U_n$ and these functions satisfy the Chebyshev equation (18.54) with $\nu = n + 1$, namely

$$(1 - x^2)V_{n+1}'' - xV_{n+1}' + (n + 1)^2 V_{n+1} = 0. \tag{18.60}$$

Evaluating the first and second derivatives of V_{n+1}, we obtain

$$V'_{n+1} = (1-x^2)^{1/2}U'_n - x(1-x^2)^{-1/2}U_n$$
$$V''_{n+1} = (1-x^2)^{1/2}U''_n - 2x(1-x^2)^{-1/2}U'_n - (1-x^2)^{-1/2}U_n - x^2(1-x^2)^{-3/2}U_n.$$

Substituting these expressions into (18.60) and dividing through by $(1-x^2)^{1/2}$, we find

$$(1-x^2)U''_n - 3xU'_n - U_n + (n+1)^2U_n = 0,$$

which immediately simplifies to give the required result (18.59). ◄

18.4.1 Properties of Chebyshev polynomials

The Chebyshev polynomials $T_n(x)$ and $U_n(x)$ have their principal applications in numerical analysis. Their use in representing other functions over the range $|x| < 1$ plays an important role in numerical integration; Gauss–Chebyshev integration is of particular value for the accurate evaluation of integrals whose integrands contain factors $(1-x^2)^{\pm 1/2}$. It is therefore worthwhile outlining some of their main properties.

Rodrigues' formula

The Chebyshev polynomials $T_n(x)$ and $U_n(x)$ may be expressed in terms of a Rodrigues' formula, in a similar way to that used for the Legendre polynomials discussed in section 18.1.2. For the Chebyshev polynomials, we have

$$T_n(x) = \frac{(-1)^n\sqrt{\pi}(1-x^2)^{1/2}}{2^n(n-\frac{1}{2})!}\frac{d^n}{dx^n}(1-x^2)^{n-\frac{1}{2}},$$
$$U_n(x) = \frac{(-1)^n\sqrt{\pi}(n+1)}{2^{n+1}(n+\frac{1}{2})!(1-x^2)^{1/2}}\frac{d^n}{dx^n}(1-x^2)^{n+\frac{1}{2}}.$$

These Rodrigues' formulae may be proved in an analogous manner to that used in section 18.1.2 when establishing the corresponding expression for the Legendre polynomials.

Mutual orthogonality

In section 17.4, we noted that Chebyshev's equation could be put into Sturm–Liouville form with $p = (1-x^2)^{1/2}$, $q = 0$, $\lambda = n^2$ and $\rho = (1-x^2)^{-1/2}$, and its natural interval is thus $[-1, 1]$. Since the Chebyshev polynomials of the first kind, $T_n(x)$, are solutions of the Chebyshev equation and are regular at the end-points $x = \pm 1$, they must be mutually orthogonal over this interval with respect to the weight function $\rho = (1-x^2)^{-1/2}$, i.e.

$$\int_{-1}^{1} T_n(x)T_m(x)(1-x^2)^{-1/2}\,dx = 0 \qquad \text{if } n \neq m. \tag{18.61}$$

The normalisation, when $m = n$, is easily found by making the substitution $x = \cos\theta$ and using (18.55). We immediately obtain

$$\int_{-1}^{1} T_n(x)T_n(x)(1-x^2)^{-1/2}\,dx = \begin{cases} \pi & \text{for } n = 0, \\ \pi/2 & \text{for } n = 1, 2, 3, \ldots . \end{cases} \tag{18.62}$$

The orthogonality and normalisation conditions mean that any (reasonable) function $f(x)$ can be expanded over the interval $|x| < 1$ in a series of the form

$$f(x) = \tfrac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n T_n(x),$$

where the coefficients in the expansion are given by

$$a_n = \frac{2}{\pi}\int_{-1}^{1} f(x)T_n(x)(1-x^2)^{-1/2}\,dx.$$

For the Chebyshev polynomials of the second kind, $U_n(x)$, we see from (18.58) that $(1-x^2)^{1/2}U_n(x) = V_{n+1}(x)$ satisfies Chebyshev's equation (18.54) with $\nu = n+1$. Thus, the orthogonality relation for the $U_n(x)$, obtained by replacing $T_i(x)$ by $V_{i+1}(x)$ in equation (18.61), reads

$$\int_{-1}^{1} U_n(x)U_m(x)(1-x^2)^{1/2}\,dx = 0 \qquad \text{if } n \neq m.$$

The corresponding normalisation condition, when $n = m$, can again be found by making the substitution $x = \cos\theta$, as illustrated in the following example.

►*Show that*

$$I \equiv \int_{-1}^{1} U_n(x)U_n(x)(1-x^2)^{1/2}\,dx = \frac{\pi}{2}.$$

From (18.58), we see that

$$I = \int_{-1}^{1} V_{n+1}(x)V_{n+1}(x)(1-x^2)^{-1/2}\,dx,$$

which, on substituting $x = \cos\theta$, gives

$$I = \int_{\pi}^{0} \sin(n+1)\theta\,\sin(n+1)\theta\,\frac{1}{\sin\theta}(-\sin\theta)\,d\theta = \frac{\pi}{2}. \blacktriangleleft$$

The above orthogonality and normalisation conditions allow one to expand any (reasonable) function in the interval $|x| < 1$ in a series of the form

$$f(x) = \sum_{n=0}^{\infty} a_n U_n(x),$$

in which the coefficients a_n are given by

$$a_n = \frac{2}{\pi}\int_{-1}^{1} f(x)U_n(x)(1-x^2)^{1/2}\,dx.$$

Generating functions

The generating functions for the Chebyshev polynomials of the first and second kinds are given, respectively, by

$$G_{\rm I}(x,h) = \frac{1-xh}{1-2xh+h^2} = \sum_{n=0}^{\infty} T_n(x)h^n, \tag{18.63}$$

$$G_{\rm II}(x,h) = \frac{1}{1-2xh+h^2} = \sum_{n=0}^{\infty} U_n(x)h^n. \tag{18.64}$$

These prescriptions may be proved in a manner similar to that used in section 18.1.2 for the generating function of the Legendre polynomials. For the Chebyshev polynomials, however, the generating functions are of less practical use, since most of the useful results can be obtained more easily by taking advantage of the trigonometric forms (18.55), as illustrated below.

Recurrence relations

There exist many useful recurrence relationships for the Chebyshev polynomials $T_n(x)$ and $U_n(x)$. They are most easily derived by setting $x = \cos\theta$ and using (18.55) and (18.58) to write

$$T_n(x) = T_n(\cos\theta) = \cos n\theta, \tag{18.65}$$

$$U_n(x) = U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta}. \tag{18.66}$$

One may then use standard formulae for the trigonometric functions to derive a wide variety of recurrence relations. Of particular use are the trigonometric identities

$$\cos(n\pm 1)\theta = \cos n\theta\,\cos\theta \mp \sin n\theta\,\sin\theta, \tag{18.67}$$

$$\sin(n\pm 1)\theta = \sin n\theta\,\cos\theta \pm \cos n\theta\,\sin\theta. \tag{18.68}$$

►*Show that the Chebyshev polynomials satisfy the recurrence relations*

$$T_{n+1}(x) - 2xT_n(x) + T_{n-1}(x) = 0, \tag{18.69}$$

$$U_{n+1}(x) - 2xU_n(x) + U_{n-1}(x) = 0. \tag{18.70}$$

Adding the result (18.67) with the plus sign to the corresponding result with a minus sign gives

$$\cos(n+1)\theta + \cos(n-1)\theta = 2\cos n\theta\,\cos\theta.$$

Using (18.65) and setting $x = \cos\theta$ immediately gives a rearrangement of the required result (18.69). Similarly, adding the plus and minus cases of result (18.68) gives

$$\sin(n+1)\theta + \sin(n-1)\theta = 2\sin n\theta\,\cos\theta.$$

Dividing through on both sides by $\sin\theta$ and using (18.66) yields (18.70). ◄

The recurrence relations (18.69) and (18.70) are extremely useful in the practical computation of Chebyshev polynomials. For example, given the values of $T_0(x)$ and $T_1(x)$ at some point x, the result (18.69) may be used iteratively to obtain the value of any $T_n(x)$ at that point; similarly, (18.70) may be used to calculate the value of any $U_n(x)$ at some point x, given the values of $U_0(x)$ and $U_1(x)$ at that point.

Further recurrence relations satisfied by the Chebyshev polynomials are

$$T_n(x) = U_n(x) - xU_{n-1}(x), \tag{18.71}$$
$$(1-x^2)U_n(x) = xT_{n+1}(x) - T_{n+2}(x), \tag{18.72}$$

which establish useful relationships between the two sets of polynomials $T_n(x)$ and $U_n(x)$. The relation (18.71) follows immediately from (18.68), whereas (18.72) follows from (18.67), with n replaced by $n+1$, on noting that $\sin^2\theta = 1 - x^2$. Additional useful results concerning the derivatives of Chebyshev polynomials may be obtained from (18.65) and (18.66), as illustrated in the following example.

►*Show that*

$$T_n'(x) = nU_{n-1}(x),$$
$$(1-x^2)U_n'(x) = xU_n(x) - (n+1)T_{n+1}(x).$$

These results are most easily derived from the expressions (18.65) and (18.66) by noting that $d/dx = (-1/\sin\theta)\,d/d\theta$. Thus,

$$T_n'(x) = -\frac{1}{\sin\theta}\frac{d(\cos n\theta)}{d\theta} = \frac{n\sin n\theta}{\sin\theta} = nU_{n-1}(x).$$

Similarly, we find

$$U_n'(x) = -\frac{1}{\sin\theta}\frac{d}{d\theta}\left[\frac{\sin(n+1)\theta}{\sin\theta}\right] = \frac{\sin(n+1)\theta\,\cos\theta}{\sin^3\theta} - \frac{(n+1)\cos(n+1)\theta}{\sin^2\theta}$$
$$= \frac{x\,U_n(x)}{1-x^2} - \frac{(n+1)T_{n+1}(x)}{1-x^2},$$

which rearranges immediately to yield the stated result. ◄

18.5 Bessel functions

Bessel's equation has the form

$$x^2y'' + xy' + (x^2 - \nu^2)y = 0, \tag{18.73}$$

which has a regular singular point at $x = 0$ and an essential singularity at $x = \infty$. The parameter ν is a given number, which we may take as ≥ 0 with no loss of generality. The equation arises from physical situations similar to those involving Legendre's equation but when cylindrical, rather than spherical, polar coordinates are employed. The variable x in Bessel's equation is usually a multiple of a radial distance and therefore ranges from 0 to ∞.

We shall seek solutions to Bessel's equation in the form of infinite series. Writing (18.73) in the standard form used in chapter 16, we have

$$y'' + \frac{1}{x}y' + \left(1 - \frac{\nu^2}{x^2}\right) y = 0. \tag{18.74}$$

By inspection, $x = 0$ is a regular singular point; hence we try a solution of the form $y = x^\sigma \sum_{n=0}^{\infty} a_n x^n$. Substituting this into (18.74) and multiplying the resulting equation by $x^{2-\sigma}$, we obtain

$$\sum_{n=0}^{\infty} \left[(\sigma + n)(\sigma + n - 1) + (\sigma + n) - \nu^2\right] a_n x^n + \sum_{n=0}^{\infty} a_n x^{n+2} = 0,$$

which simplifies to

$$\sum_{n=0}^{\infty} \left[(\sigma + n)^2 - \nu^2\right] a_n x^n + \sum_{n=0}^{\infty} a_n x^{n+2} = 0.$$

Considering the coefficient of x^0, we obtain the indicial equation

$$\sigma^2 - \nu^2 = 0,$$

and so $\sigma = \pm\nu$. For coefficients of higher powers of x we find

$$\left[(\sigma + 1)^2 - \nu^2\right] a_1 = 0, \tag{18.75}$$

$$\left[(\sigma + n)^2 - \nu^2\right] a_n + a_{n-2} = 0 \qquad \text{for } n \geq 2. \tag{18.76}$$

Substituting $\sigma = \pm\nu$ into (18.75) and (18.76), we obtain the recurrence relations

$$(1 \pm 2\nu)a_1 = 0, \tag{18.77}$$

$$n(n \pm 2\nu)a_n + a_{n-2} = 0 \qquad \text{for } n \geq 2. \tag{18.78}$$

We consider now the form of the general solution to Bessel's equation (18.73) for two cases: the case for which ν is not an integer and that for which it is (including zero).

18.5.1 Bessel functions for non-integer ν

If ν is a non-integer then, in general, the two roots of the indicial equation, $\sigma_1 = \nu$ and $\sigma_2 = -\nu$, will not differ by an integer, and we may obtain two linearly independent solutions in the form of Frobenius series. Special considerations do arise, however, when $\nu = m/2$ for $m = 1, 3, 5, \ldots$, and $\sigma_1 - \sigma_2 = 2\nu = m$ is an (odd positive) integer. When this happens, we may always obtain a solution in the form of a Frobenius series corresponding to the larger root, $\sigma_1 = \nu = m/2$, as described above. However, for the smaller root, $\sigma_2 = -\nu = -m/2$, we must determine whether a second Frobenius series solution is possible by examining the recurrence relation (18.78), which reads

$$n(n-m)a_n + a_{n-2} = 0 \qquad \text{for } n \geq 2.$$

Since m is an *odd* positive integer in this case, we can use this recurrence relation (starting with $a_0 \neq 0$) to calculate $a_2, a_4, a_6, \ldots$ in the knowledge that all these terms will remain finite. It is possible in this case, therefore, to find a second solution in the form of a Frobenius series, one that corresponds to the smaller root σ_2.

Thus, in general, for non-integer ν we have from (18.77) and (18.78)

$$\begin{aligned} a_n &= -\frac{1}{n(n \pm 2\nu)} a_{n-2} \qquad \text{for } n = 2, 4, 6, \ldots, \\ &= 0 \qquad \text{for } n = 1, 3, 5, \ldots. \end{aligned}$$

Setting $a_0 = 1$ in each case, we obtain the two solutions

$$y_{\pm\nu}(x) = x^{\pm\nu} \left[1 - \frac{x^2}{2(2 \pm 2\nu)} + \frac{x^4}{2 \times 4(2 \pm 2\nu)(4 \pm 2\nu)} - \cdots \right].$$

It is customary, however, to set

$$a_0 = \frac{1}{2^{\pm\nu}\Gamma(1 \pm \nu)},$$

where $\Gamma(x)$ is the *gamma function*, described in subsection 18.12.1; it may be regarded as the generalisation of the factorial function to non-integer and/or negative arguments.§ The two solutions of (18.73) are then written as $J_\nu(x)$ and $J_{-\nu}(x)$, where

$$\begin{aligned} J_\nu(x) &= \frac{1}{\Gamma(\nu+1)} \left(\frac{x}{2}\right)^\nu \left[1 - \frac{1}{\nu+1} \left(\frac{x}{2}\right)^2 + \frac{1}{(\nu+1)(\nu+2)} \frac{1}{2!} \left(\frac{x}{2}\right)^4 - \cdots \right] \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\Gamma(\nu+n+1)} \left(\frac{x}{2}\right)^{\nu+2n}; \end{aligned} \tag{18.79}$$

replacing ν by $-\nu$ gives $J_{-\nu}(x)$. The functions $J_\nu(x)$ and $J_{-\nu}(x)$ are called *Bessel functions of the first kind, of order* ν. Since the first term of each series is a finite non-zero multiple of x^ν and $x^{-\nu}$, respectively, if ν is not an integer then $J_\nu(x)$ and $J_{-\nu}(x)$ are linearly independent. This may be confirmed by calculating the Wronskian of these two functions. Therefore, for non-integer ν the general solution of Bessel's equation (18.73) is given by

$$y(x) = c_1 J_\nu(x) + c_2 J_{-\nu}(x). \tag{18.80}$$

§ In particular, $\Gamma(n+1) = n!$ for $n = 0, 1, 2, \ldots$, and $\Gamma(n)$ is infinite if n is any integer ≤ 0.

We note that Bessel functions of half-integer order are expressible in closed form in terms of trigonometric functions, as illustrated in the following example.

►*Find the general solution of*

$$x^2y'' + xy' + (x^2 - \tfrac{1}{4})y = 0.$$

This is Bessel's equation with $\nu = 1/2$, so from (18.80) the general solution is simply

$$y(x) = c_1 J_{1/2}(x) + c_2 J_{-1/2}(x).$$

However, Bessel functions of half-integral order can be expressed in terms of trigonometric functions. To show this, we note from (18.79) that

$$J_{\pm 1/2}(x) = x^{\pm 1/2} \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{2^{2n\pm 1/2} n!\,\Gamma(1 + n \pm \frac{1}{2})}.$$

Using the fact that $\Gamma(x+1) = x\Gamma(x)$ and $\Gamma(\frac{1}{2}) = \sqrt{\pi}$, we find that, for $\nu = 1/2$,

$$\begin{aligned}
J_{1/2}(x) &= \frac{(\frac{1}{2}x)^{1/2}}{\Gamma(\frac{3}{2})} - \frac{(\frac{1}{2}x)^{5/2}}{1!\,\Gamma(\frac{5}{2})} + \frac{(\frac{1}{2}x)^{9/2}}{2!\,\Gamma(\frac{7}{2})} - \cdots \\
&= \frac{(\frac{1}{2}x)^{1/2}}{(\frac{1}{2})\sqrt{\pi}} - \frac{(\frac{1}{2}x)^{5/2}}{1!(\frac{3}{2})(\frac{1}{2})\sqrt{\pi}} + \frac{(\frac{1}{2}x)^{9/2}}{2!(\frac{5}{2})(\frac{3}{2})(\frac{1}{2})\sqrt{\pi}} - \cdots \\
&= \frac{(\frac{1}{2}x)^{1/2}}{(\frac{1}{2})\sqrt{\pi}} \left(1 - \frac{x^2}{3!} + \frac{x^4}{5!} - \cdots\right) = \frac{(\frac{1}{2}x)^{1/2}}{(\frac{1}{2})\sqrt{\pi}} \frac{\sin x}{x} = \sqrt{\frac{2}{\pi x}}\sin x,
\end{aligned}$$

whereas for $\nu = -1/2$ we obtain

$$\begin{aligned}
J_{-1/2}(x) &= \frac{(\frac{1}{2}x)^{-1/2}}{\Gamma(\frac{1}{2})} - \frac{(\frac{1}{2}x)^{3/2}}{1!\,\Gamma(\frac{3}{2})} + \frac{(\frac{1}{2}x)^{7/2}}{2!\,\Gamma(\frac{5}{2})} - \cdots \\
&= \frac{(\frac{1}{2}x)^{-1/2}}{\sqrt{\pi}} \left(1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \cdots\right) = \sqrt{\frac{2}{\pi x}}\cos x.
\end{aligned}$$

Therefore the general solution we require is

$$y(x) = c_1 J_{1/2}(x) + c_2 J_{-1/2}(x) = c_1\sqrt{\frac{2}{\pi x}}\sin x + c_2\sqrt{\frac{2}{\pi x}}\cos x. \blacktriangleleft$$

18.5.2 Bessel functions for integer ν

The definition of the Bessel function $J_\nu(x)$ given in (18.79) is, of course, valid for all values of ν, but, as we shall see, in the case of integer ν the general solution of Bessel's equation cannot be written in the form (18.80). Firstly, let us consider the case $\nu = 0$, so that the two solutions to the indicial equation are equal, and we clearly obtain only one solution in the form of a Frobenius series. From (18.79),

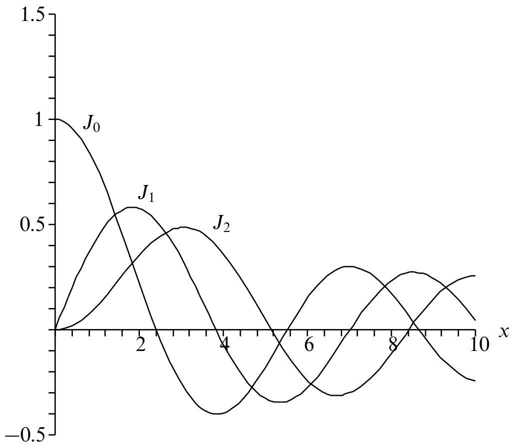

Figure 18.5 The first three integer-order Bessel functions of the first kind.

this is given by

$$J_0(x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{2^{2n} n! \Gamma(1+n)}$$
$$= 1 - \frac{x^2}{2^2} + \frac{x^4}{2^2 4^2} - \frac{x^6}{2^2 4^2 6^2} + \cdots .$$

In general, however, if ν is a positive integer then the solutions of the indicial equation differ by an integer. For the larger root, $\sigma_1 = \nu$, we may find a solution $J_\nu(x)$, for $\nu = 1, 2, 3, \ldots$, in the form of the Frobenius series given by (18.79). Graphs of $J_0(x)$, $J_1(x)$ and $J_2(x)$ are plotted in figure 18.5 for real x. For the smaller root, $\sigma_2 = -\nu$, however, the recurrence relation (18.78) becomes

$$n(n-m)a_n + a_{n-2} = 0 \qquad \text{for } n \geq 2,$$

where $m = 2\nu$ is now an *even* positive integer, i.e. $m = 2, 4, 6, \ldots$. Starting with $a_0 \neq 0$ we may then calculate $a_2, a_4, a_6, \ldots$, but we see that when $n = m$ the coefficient a_n is formally infinite, and the method fails to produce a second solution in the form of a Frobenius series.

In fact, by replacing ν by $-\nu$ in the definition of $J_\nu(x)$ given in (18.79), it can be shown that, for integer ν,

$$J_{-\nu}(x) = (-1)^\nu J_\nu(x),$$

and hence that $J_\nu(x)$ and $J_{-\nu}(x)$ are linearly dependent. So, in this case, we cannot write the general solution to Bessel's equation in the form (18.80). One therefore defines the function

$$Y_\nu(x) = \frac{J_\nu(x)\cos\nu\pi - J_{-\nu}(x)}{\sin\nu\pi}, \tag{18.81}$$

which is called a Bessel function of the *second kind* of order ν (or, occasionally, a *Weber* or *Neumann* function). As Bessel's equation is linear, $Y_\nu(x)$ is clearly a solution, since it is just the weighted sum of Bessel functions of the first kind. Furthermore, for non-integer ν it is clear that $Y_\nu(x)$ is linearly independent of $J_\nu(x)$. It may also be shown that the Wronskian of $J_\nu(x)$ and $Y_\nu(x)$ is non-zero for *all* values of ν. Hence $J_\nu(x)$ and $Y_\nu(x)$ always constitute a pair of independent solutions.

►*If n is an integer, show that $Y_{n+1/2}(x) = (-1)^{n+1}J_{-n-1/2}(x)$.*

From (18.81), we have

$$Y_{n+1/2}(x) = \frac{J_{n+1/2}(x)\cos(n+\frac{1}{2})\pi - J_{-n-1/2}(x)}{\sin(n+\frac{1}{2})\pi}.$$

If n is an integer, $\cos(n+\frac{1}{2})\pi = 0$ and $\sin(n+\frac{1}{2})\pi = (-1)^n$, and so we immediately obtain $Y_{n+1/2}(x) = (-1)^{n+1}J_{-n-1/2}(x)$, as required. ◄

The expression (18.81) becomes an indeterminate form 0/0 when ν is an integer, however. This is so because for integer ν we have $\cos\nu\pi = (-1)^\nu$ and $J_{-\nu}(x) = (-1)^\nu J_\nu(x)$. Nevertheless, this indeterminate form can be evaluated using l'Hôpital's rule (see chapter 4). Therefore, for integer ν, we set

$$Y_\nu(x) = \lim_{\mu\to\nu}\left[\frac{J_\mu(x)\cos\mu\pi - J_{-\mu}(x)}{\sin\mu\pi}\right], \tag{18.82}$$

which gives a linearly independent second solution for this case. Thus, we may write the general solution of Bessel's equation, valid for *all* ν, as

$$y(x) = c_1 J_\nu(x) + c_2 Y_\nu(x). \tag{18.83}$$

The functions $Y_0(x)$, $Y_1(x)$ and $Y_2(x)$ are plotted in figure 18.6

Finally, we note that, in some applications, it is convenient to work with complex linear combinations of Bessel functions of the first and second kinds given by

$$H_\nu^{(1)}(x) = J_\nu(x) + iY_\nu(x), \qquad H_\nu^{(2)}(x) = J_\nu(x) - iY_\nu(x);$$

these are called, respectively, *Hankel functions* of the first and second kind of order ν.

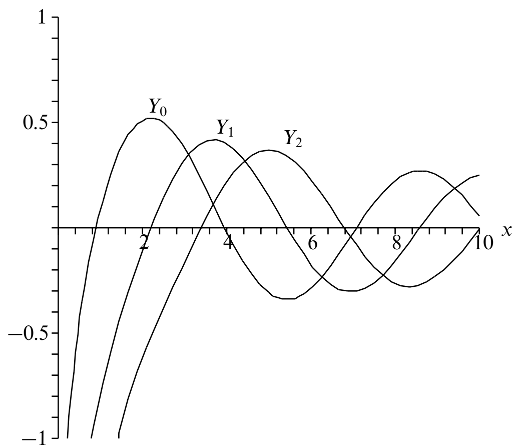

Figure 18.6 The first three integer-order Bessel functions of the second kind.

18.5.3 Properties of Bessel functions $J_\nu(x)$

In physical applications, we often require that the solution is regular at $x = 0$, but, from its definition (18.81) or (18.82), it is clear that $Y_\nu(x)$ is singular at the origin, and so in such physical situations the coefficient c_2 in (18.83) must be set to zero; the solution is then simply some multiple of $J_\nu(x)$. These Bessel functions of the first kind have various useful properties that are worthy of further discussion. Unless otherwise stated, the results presented in this section apply to Bessel functions $J_\nu(x)$ of integer and non-integer order.

Mutual orthogonality

In section 17.4, we noted that Bessel's equation (18.73) could be put into conventional Sturm–Liouville form with $p = x$, $q = -\nu^2/x$, $\lambda = \alpha^2$ and $\rho = x$, provided αx is the argument of y. From the form of p, we see that there is no natural interval over which one would expect the solutions of Bessel's equation corresponding to different eigenvalues λ (but fixed ν) to be automatically orthogonal. Nevertheless, provided the Bessel functions satisfied appropriate boundary conditions, we would expect them to obey an orthogonality relationship over some interval $[a, b]$ of the form

$$\int_a^b xJ_\nu(\alpha x)J_\nu(\beta x)\,dx = 0 \qquad \text{for } \alpha \neq \beta. \tag{18.84}$$

To determine the required boundary conditions for this result to hold, let us consider the functions $f(x) = J_\nu(\alpha x)$ and $g(x) = J_\nu(\beta x)$, which, as will be proved below, respectively satisfy the equations

$$x^2 f'' + xf' + (\alpha^2 x^2 - \nu^2)f = 0, \tag{18.85}$$
$$x^2 g'' + xg' + (\beta^2 x^2 - \nu^2)g = 0. \tag{18.86}$$

►*Show that $f(x) = J_\nu(\alpha x)$ satisfies (18.85).*

If $f(x) = J_\nu(\alpha x)$ and we write $w = \alpha x$, then

$$\frac{df}{dx} = \alpha \frac{dJ_\nu(w)}{dw} \qquad \text{and} \qquad \frac{d^2 f}{dx^2} = \alpha^2 \frac{d^2 J_\nu(w)}{dw^2}.$$

When these expressions are substituted into (18.85), its LHS becomes

$$x^2\alpha^2 \frac{d^2 J_\nu(w)}{dw^2} + x\alpha \frac{dJ_\nu(w)}{dw} + (\alpha^2 x^2 - \nu^2)J_\nu(w)$$
$$= w^2 \frac{d^2 J_\nu(w)}{dw^2} + w\frac{dJ_\nu(w)}{dw} + (w^2 - \nu^2)J_\nu(w).$$

But, from Bessel's equation itself, this final expression is equal to zero, thus verifying that $f(x)$ does satisfy (18.85). ◄

Now multiplying (18.86) by $f(x)$ and (18.85) by $g(x)$ and subtracting them gives

$$\frac{d}{dx}[x(fg' - gf')] = (\alpha^2 - \beta^2)xfg, \tag{18.87}$$

where we have used the fact that

$$\frac{d}{dx}[x(fg' - gf')] = x(fg'' - gf'') + (fg' - gf').$$

By integrating (18.87) over any given range $x = a$ to $x = b$, we obtain

$$\int_a^b xf(x)g(x)\,dx = \frac{1}{\alpha^2 - \beta^2}\Big[xf(x)g'(x) - xg(x)f'(x)\Big]_a^b,$$

which, on setting $f(x) = J_\nu(\alpha x)$ and $g(x) = J_\nu(\beta x)$, becomes

$$\int_a^b xJ_\nu(\alpha x)J_\nu(\beta x)\,dx = \frac{1}{\alpha^2 - \beta^2}\Big[\beta x J_\nu(\alpha x)J_\nu'(\beta x) - \alpha x J_\nu(\beta x)J_\nu'(\alpha x)\Big]_a^b. \tag{18.88}$$

If $\alpha \neq \beta$, and the interval $[a, b]$ is such that the expression on the RHS of (18.88) equals zero, then we obtain the orthogonality condition (18.84). This happens, for example, if $J_\nu(\alpha x)$ and $J_\nu(\beta x)$ vanish at $x = a$ and $x = b$, or if $J_\nu'(\alpha x)$ and $J_\nu'(\beta x)$ vanish at $x = a$ and $x = b$, or for many more general conditions. It should be noted that the boundary term is automatically zero at the point $x = 0$, as one might expect from the fact that the Sturm–Liouville form of Bessel's equation has $p(x) = x$.

If $\alpha = \beta$, the RHS of (18.88) takes the indeterminant form 0/0. This may be evaluated using l'Hôpital's rule, or alternatively we may calculate the relevant integral directly.

►*Evaluate the integral*

$$\int_a^b J_\nu^2(\alpha x)x\,dx.$$

Ignoring the integration limits for the moment,

$$\int J_\nu^2(\alpha x)x\,dx = \frac{1}{\alpha^2}\int J_\nu^2(u)u\,du,$$

where $u = \alpha x$. Integrating by parts yields

$$I = \int J_\nu^2(u)u\,du = \tfrac{1}{2}u^2 J_\nu^2(u) - \int J_\nu(u)J_\nu'(u)u^2\,du.$$

Now Bessel's equation (18.73) can be rearranged as

$$u^2 J_\nu(u) = \nu^2 J_\nu(u) - uJ_\nu'(u) - u^2 J_\nu''(u),$$

which, on substitution into the expression for I, gives

$$\begin{aligned} I &= \tfrac{1}{2}u^2 J_\nu^2(u) - \int J_\nu'(u)[\nu^2 J_\nu(u) - uJ_\nu'(u) - u^2 J_\nu''(u)]\,du \\ &= \tfrac{1}{2}u^2 J_\nu^2(u) - \tfrac{1}{2}\nu^2 J_\nu^2(u) + \tfrac{1}{2}u^2[J_\nu'(u)]^2 + c. \end{aligned}$$

Since $u = \alpha x$, the required integral is given by

$$\int_a^b J_\nu^2(\alpha x)x\,dx = \frac{1}{2}\left[\left(x^2 - \frac{\nu^2}{\alpha^2}\right)J_\nu^2(\alpha x) + x^2[J_\nu'(\alpha x)]^2\right]_a^b, \qquad (18.89)$$

which gives the normalisation condition for Bessel functions of the first kind. ◄

Since the Bessel functions $J_\nu(x)$ possess the orthogonality property (18.88), we may expand any reasonable function $f(x)$, i.e. one obeying the Dirichlet conditions discussed in chapter 12, in the interval $0 \le x \le b$ as a sum of Bessel functions of a given (non-negative) order ν,

$$f(x) = \sum_{n=0}^{\infty} c_n J_\nu(\alpha_n x), \qquad (18.90)$$

provided that the α_n are chosen such that $J_\nu(\alpha_n b) = 0$. The coefficients c_n are then given by

$$c_n = \frac{2}{b^2 J_{\nu+1}^2(\alpha_n b)}\int_0^b f(x)J_\nu(\alpha_n x)x\,dx. \qquad (18.91)$$

The interval is taken to be $0 \le x \le b$, as then one need only ensure that the appropriate boundary condition is satisfied at $x = b$, since the boundary condition at $x = 0$ is met automatically.

►*Prove the expression (18.91).*

If we multiply (18.90) by $xJ_\nu(\alpha_m x)$ and integrate from $x = 0$ to $x = b$ then we obtain

$$\begin{aligned}\int_0^b xJ_\nu(\alpha_m x)f(x)\,dx &= \sum_{n=0}^{\infty} c_n \int_0^b xJ_\nu(\alpha_m x)J_\nu(\alpha_n x)\,dx \\ &= c_m \int_0^b J_\nu^2(\alpha_m x)x\,dx \\ &= \tfrac{1}{2}c_m b^2 J'^2_\nu(\alpha_m b) = \tfrac{1}{2}c_m b^2 J_{\nu+1}^2(\alpha_m b),\end{aligned}$$

where in the last two lines we have used (18.88) with $\alpha_m = \alpha \neq \beta = \alpha_n$, (18.89), the fact that $J_\nu(\alpha_m b) = 0$ and (18.95), which is proved below. ◄

Recurrence relations

The recurrence relations enjoyed by Bessel functions of the first kind, $J_\nu(x)$, can be derived directly from the power series definition (18.79).

►*Prove the recurrence relation*

$$\frac{d}{dx}[x^\nu J_\nu(x)] = x^\nu J_{\nu-1}(x). \tag{18.92}$$

From the power series definition (18.79) of $J_\nu(x)$ we obtain

$$\begin{aligned}\frac{d}{dx}[x^\nu J_\nu(x)] &= \frac{d}{dx}\sum_{n=0}^{\infty} \frac{(-1)^n x^{2\nu+2n}}{2^{\nu+2n} n!\Gamma(\nu+n+1)} \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n x^{2\nu+2n-1}}{2^{\nu+2n-1} n!\Gamma(\nu+n)} \\ &= x^\nu \sum_{n=0}^{\infty} \frac{(-1)^n x^{(\nu-1)+2n}}{2^{(\nu-1)+2n} n!\Gamma((\nu-1)+n+1)} = x^\nu J_{\nu-1}(x). \; ◄\end{aligned}$$

It may similarly be shown that

$$\frac{d}{dx}[x^{-\nu} J_\nu(x)] = -x^{-\nu} J_{\nu+1}(x). \tag{18.93}$$

From (18.92) and (18.93) the remaining recurrence relations may be derived. Expanding out the derivative on the LHS of (18.92) and dividing through by $x^{\nu-1}$, we obtain the relation

$$xJ'_\nu(x) + \nu J_\nu(x) = xJ_{\nu-1}(x). \tag{18.94}$$

Similarly, by expanding out the derivative on the LHS of (18.93), and multiplying through by $x^{\nu+1}$, we find

$$xJ'_\nu(x) - \nu J_\nu(x) = -xJ_{\nu+1}(x). \tag{18.95}$$

Adding (18.94) and (18.95) and dividing through by x gives

$$J_{\nu-1}(x) - J_{\nu+1}(x) = 2J'_\nu(x). \tag{18.96}$$

Finally, subtracting (18.95) from (18.94) and dividing by x gives

$$J_{\nu-1}(x) + J_{\nu+1}(x) = \frac{2\nu}{x} J_\nu(x). \tag{18.97}$$

►*Given that $J_{1/2}(x) = (2/\pi x)^{1/2} \sin x$ and that $J_{-1/2}(x) = (2/\pi x)^{1/2} \cos x$, express $J_{3/2}(x)$ and $J_{-3/2}(x)$ in terms of trigonometric functions.*

From (18.95) we have

$$\begin{aligned}
J_{3/2}(x) &= \frac{1}{2x} J_{1/2}(x) - J'_{1/2}(x) \\
&= \frac{1}{2x}\left(\frac{2}{\pi x}\right)^{1/2} \sin x - \left(\frac{2}{\pi x}\right)^{1/2} \cos x + \frac{1}{2x}\left(\frac{2}{\pi x}\right)^{1/2} \sin x \\
&= \left(\frac{2}{\pi x}\right)^{1/2} \left(\frac{1}{x} \sin x - \cos x\right).
\end{aligned}$$

Similarly, from (18.94) we have

$$\begin{aligned}
J_{-3/2}(x) &= -\frac{1}{2x} J_{-1/2}(x) + J'_{-1/2}(x) \\
&= -\frac{1}{2x}\left(\frac{2}{\pi x}\right)^{1/2} \cos x - \left(\frac{2}{\pi x}\right)^{1/2} \sin x - \frac{1}{2x}\left(\frac{2}{\pi x}\right)^{1/2} \cos x \\
&= \left(\frac{2}{\pi x}\right)^{1/2} \left(-\frac{1}{x} \cos x - \sin x\right).
\end{aligned}$$

We see that, by repeated use of these recurrence relations, all Bessel functions $J_\nu(x)$ of half-integer order may be expressed in terms of trigonometric functions. From their definition (18.81), Bessel functions of the second kind, $Y_\nu(x)$, of half-integer order can be similarly expressed. ◄

Finally, we note that the relations (18.92) and (18.93) may be rewritten in integral form as

$$\begin{aligned}
\int x^\nu J_{\nu-1}(x)\, dx &= x^\nu J_\nu(x), \\
\int x^{-\nu} J_{\nu+1}(x)\, dx &= -x^{-\nu} J_\nu(x).
\end{aligned}$$

If ν is an integer, the recurrence relations of this section may be proved using the generating function for Bessel functions discussed below. It may be shown that Bessel functions of the second kind, $Y_\nu(x)$, also satisfy the recurrence relations derived above.

Generating function

The Bessel functions $J_\nu(x)$, where $\nu = n$ is an integer, can be described by a generating function in a way similar to that discussed for Legendre polynomials in subsection 18.1.2. The generating function for Bessel functions of integer order is given by

$$G(x,h) = \exp\left[\frac{x}{2}\left(h - \frac{1}{h}\right)\right] = \sum_{n=-\infty}^{\infty} J_n(x)h^n. \tag{18.98}$$

By expanding the exponential as a power series, it is straightfoward to verify that the functions $J_n(x)$ defined by (18.98) are indeed Bessel functions of the first kind, as given by (18.79).

The generating function (18.98) is useful for finding, for Bessel functions of integer order, properties that can often be extended to the non-integer case. In particular, the Bessel function recurrence relations may be derived.

►*Use the generating function to prove, for integer ν, the recurrence relation (18.97), i.e.*

$$J_{\nu-1}(x) + J_{\nu+1}(x) = \frac{2\nu}{x}J_\nu(x).$$

Differentiating $G(x,h)$ with respect to h we obtain

$$\frac{\partial G(x,h)}{\partial h} = \frac{x}{2}\left(1 + \frac{1}{h^2}\right)G(x,h) = \sum_{n=-\infty}^{\infty} nJ_n(x)h^{n-1},$$

which can be written using (18.98) again as

$$\frac{x}{2}\left(1 + \frac{1}{h^2}\right)\sum_{n=-\infty}^{\infty} J_n(x)h^n = \sum_{n=-\infty}^{\infty} nJ_n(x)h^{n-1}.$$

Equating coefficients of h^n we obtain

$$\frac{x}{2}[J_n(x) + J_{n+2}(x)] = (n+1)J_{n+1}(x),$$

which, on replacing n by $\nu - 1$, gives the required recurrence relation. ◄

Integral representations

The generating function (18.98) is also useful for deriving *integral representations* of Bessel functions of integer order.

►*Show that for integer n the Bessel function $J_n(x)$ is given by*

$$J_n(x) = \frac{1}{\pi}\int_0^\pi \cos(n\theta - x\sin\theta)\,d\theta. \tag{18.99}$$

By expanding out the cosine term in the integrand in (18.99) we obtain the integral

$$I = \frac{1}{\pi}\int_0^\pi [\cos(x\sin\theta)\cos n\theta + \sin(x\sin\theta)\sin n\theta]\,d\theta. \tag{18.100}$$

Now, we may express $\cos(x\sin\theta)$ and $\sin(x\sin\theta)$ in terms of Bessel functions by setting $h = \exp i\theta$ in (18.98) to give

$$\exp\left[\frac{x}{2}(\exp i\theta - \exp(-i\theta))\right] = \exp(ix\sin\theta) = \sum_{m=-\infty}^{\infty} J_m(x)\exp im\theta.$$

Using de Moivre's theorem, $\exp i\theta = \cos\theta + i\sin\theta$, we then obtain

$$\exp(ix\sin\theta) = \cos(x\sin\theta) + i\sin(x\sin\theta) = \sum_{m=-\infty}^{\infty} J_m(x)(\cos m\theta + i\sin m\theta).$$

Equating the real and imaginary parts of this expression gives

$$\cos(x\sin\theta) = \sum_{m=-\infty}^{\infty} J_m(x)\cos m\theta,$$

$$\sin(x\sin\theta) = \sum_{m=-\infty}^{\infty} J_m(x)\sin m\theta.$$

Substituting these expressions into (18.100) then yields

$$I = \frac{1}{\pi}\sum_{m=-\infty}^{\infty}\int_0^{\pi}[J_m(x)\cos m\theta\cos n\theta + J_m(x)\sin m\theta\sin n\theta]\,d\theta.$$

However, using the orthogonality of the trigonometric functions [see equations (12.1)–(12.3)], we obtain

$$I = \frac{1}{\pi}\frac{\pi}{2}[J_n(x) + J_n(x)] = J_n(x),$$

which proves the integral representation (18.99). ◀

Finally, we mention the special case of the integral representation (18.99) for $n = 0$:

$$J_0(x) = \frac{1}{\pi}\int_0^{\pi}\cos(x\sin\theta)\,d\theta = \frac{1}{2\pi}\int_0^{2\pi}\cos(x\sin\theta)\,d\theta,$$

since $\cos(x\sin\theta)$ repeats itself in the range $\theta = \pi$ to $\theta = 2\pi$. However, $\sin(x\sin\theta)$ changes sign in this range and so

$$\frac{1}{2\pi}\int_0^{2\pi}\sin(x\sin\theta)\,d\theta = 0.$$

Using de Moivre's theorem, we can therefore write

$$J_0(x) = \frac{1}{2\pi}\int_0^{2\pi}\exp(ix\sin\theta)\,d\theta = \frac{1}{2\pi}\int_0^{2\pi}\exp(ix\cos\theta)\,d\theta.$$

There are in fact many other integral representations of Bessel functions; they can be derived from those given.

18.6 Spherical Bessel functions

When obtaining solutions of Helmholtz' equation $(\nabla^2 + k^2)u = 0$ in spherical polar coordinates (see section 21.3.2), one finds that, for solutions that are finite on the polar axis, the radial part $R(r)$ of the solution must satisfy the equation

$$r^2R'' + 2rR' + [k^2r^2 - \ell(\ell+1)]R = 0, \qquad (18.101)$$

where ℓ is an integer. This equation looks very much like Bessel's equation and can in fact be reduced to it by writing $R(r) = r^{-1/2}S(r)$, in which case $S(r)$ then satisfies

$$r^2 S'' + rS' + \left[k^2r^2 - \left(\ell + \tfrac{1}{2}\right)^2\right] S = 0.$$

On making the change of variable $x = kr$ and letting $y(x) = S(kr)$, we obtain

$$x^2 y'' + xy' + [x^2 - (\ell + \tfrac{1}{2})^2]y = 0,$$

where the primes now denote d/dx. This is Bessel's equation of order $\ell + \frac{1}{2}$ and has as its solutions $y(x) = J_{\ell+1/2}(x)$ and $Y_{\ell+1/2}(x)$. The general solution of (18.101) can therefore be written

$$R(r) = r^{-1/2}[c_1 J_{\ell+1/2}(kr) + c_2 Y_{\ell+1/2}(kr)],$$

where c_1 and c_2 are constants that may be determined from the boundary conditions on the solution. In particular, for solutions that are finite at the origin we require $c_2 = 0$.

The functions $x^{-1/2}J_{\ell+1/2}(x)$ and $x^{-1/2}Y_{\ell+1/2}(x)$, when suitably normalised, are called *spherical Bessel functions* of the first and second kind, respectively, and are denoted as follows:

$$j_\ell(x) = \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x), \qquad (18.102)$$

$$n_\ell(x) = \sqrt{\frac{\pi}{2x}} Y_{\ell+1/2}(x). \qquad (18.103)$$

For integer ℓ, we also note that $Y_{\ell+1/2}(x) = (-1)^{\ell+1}J_{-\ell-1/2}(x)$, as discussed in section 18.5.2. Moreover, in section 18.5.1, we noted that Bessel functions of the first kind, $J_\nu(x)$, of half-integer order are expressible in closed form in terms of trigonometric functions. Thus, all spherical Bessel functions of both the first and second kinds may be expressed in such a form. In particular, using the results of the worked example in section 18.5.1, we find that

$$j_0(x) = \frac{\sin x}{x}, \qquad (18.104)$$

$$n_0(x) = -\frac{\cos x}{x}. \qquad (18.105)$$

Expressions for higher-order spherical Bessel functions are most easily obtained by using the recurrence relations for Bessel functions.

►*Show that the ℓth spherical Bessel function is given by*

$$f_\ell(x) = (-1)^\ell x^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell f_0(x), \tag{18.106}$$

where $f_\ell(x)$ denotes either $j_\ell(x)$ or $n_\ell(x)$.

The recurrence relation (18.93) for Bessel functions of the first kind reads

$$J_{\nu+1}(x) = -x^\nu \frac{d}{dx}\left[x^{-\nu}J_\nu(x)\right].$$

Thus, on setting $\nu = \ell + \frac{1}{2}$ and rearranging, we find

$$x^{-1/2}J_{\ell+3/2}(x) = -x^\ell \frac{d}{dx}\left[\frac{x^{-1/2}J_{\ell+1/2}}{x^\ell}\right],$$

which on using (18.102) yields the recurrence relation

$$j_{\ell+1}(x) = -x^\ell \frac{d}{dx}[x^{-\ell} j_\ell(x)].$$

We now change $\ell + 1 \to \ell$ and iterate this result:

$$\begin{aligned}
j_\ell(x) &= -x^{\ell-1}\frac{d}{dx}[x^{-\ell+1}j_{\ell-1}(x)] \\
&= -x^{\ell-1}\frac{d}{dx}\left\{x^{-\ell+1}(-1)x^{\ell-2}\frac{d}{dx}\left[x^{-\ell+2}j_{\ell-2}(x)\right]\right\} \\
&= (-1)^2\frac{x^\ell}{x}\frac{d}{dx}\left\{\frac{1}{x}\frac{d}{dx}\left[x^{-\ell+2}j_{\ell-2}(x)\right]\right\} \\
&= \cdots \\
&= (-1)^\ell x^\ell\left(\frac{1}{x}\frac{d}{dx}\right)^\ell j_0(x).
\end{aligned}$$

This is the expression for $j_\ell(x)$ as given in (18.106). One may prove the result (18.106) for $n_\ell(x)$ in an analogous manner by setting $\nu = \ell - \frac{1}{2}$ in the recurrence relation (18.92) for Bessel functions of the first kind and using the relationship $Y_{\ell+1/2}(x) = (-1)^{\ell+1}J_{-\ell-1/2}(x)$. ◄

Using result (18.106) and the expressions (18.104) and (18.105), one quickly finds, for example,

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}, \qquad j_2(x) = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3\cos x}{x^2},$$

$$n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}, \qquad n_2(x) = -\left(\frac{3}{x^3} - \frac{1}{x}\right)\cos x - \frac{3\sin x}{x^2}.$$

Finally, we note that the orthogonality properties of the spherical Bessel functions follow directly from the orthogonality condition (18.88) for Bessel functions of the first kind.

18.7 Laguerre functions

Laguerre's equation has the form

$$xy'' + (1-x)y' + \nu y = 0; \tag{18.107}$$

it has a regular singularity at $x = 0$ and an essential singularity at $x = \infty$. The parameter ν is a given real number, although it nearly always takes an integer value in physical applications. The Laguerre equation appears in the description of the wavefunction of the hydrogen atom. Any solution of (18.107) is called a *Laguerre function*.

Since the point $x = 0$ is a regular singularity, we may find at least one solution in the form of a Frobenius series (see section 16.3):

$$y(x) = \sum_{m=0}^{\infty} a_m x^{m+\sigma}. \tag{18.108}$$

Substituting this series into (18.107) and dividing through by $x^{\sigma-1}$, we obtain

$$\sum_{m=0}^{\infty} \left[(m+\sigma)(m+\sigma-1) + (1-x)(m+\sigma) + \nu x\right] a_m x^m = 0. \tag{18.109}$$

Setting $x = 0$, so that only the $m = 0$ term remains, we obtain the indicial equation $\sigma^2 = 0$, which trivially has $\sigma = 0$ as its repeated root. Thus, Laguerre's equation has only one solution of the form (18.108), and it, in fact, reduces to a simple power series. Substituting $\sigma = 0$ into (18.109) and demanding that the coefficient of x^{m+1} vanishes, we obtain the recurrence relation

$$a_{m+1} = \frac{m-\nu}{(m+1)^2} a_m.$$

As mentioned above, in nearly all physical applications, the parameter ν takes integer values. Therefore, if $\nu = n$, where n is a non-negative integer, we see that $a_{n+1} = a_{n+2} = \cdots = 0$, and so our solution to Laguerre's equation is a polynomial of order n. It is conventional to choose $a_0 = 1$, so that the solution is given by

$$L_n(x) = \frac{(-1)^n}{n!}\left[x^n - \frac{n^2}{1!}x^{n-1} + \frac{n^2(n-1)^2}{2!}x^{n-2} - \cdots + (-1)^n n!\right] \tag{18.110}$$

$$= \sum_{m=0}^{n} (-1)^m \frac{n!}{(m!)^2(n-m)!} x^m, \tag{18.111}$$

where $L_n(x)$ is called the nth *Laguerre polynomial*. We note in particular that $L_n(0) = 1$. The first few Laguerre polynomials are given by

$$\begin{aligned}
&L_0(x) = 1, && 3!L_3(x) = -x^3 + 9x^2 - 18x + 6,\\
&L_1(x) = -x + 1, && 4!L_4(x) = x^4 - 16x^3 + 72x^2 - 96x + 24,\\
&2!L_2(x) = x^2 - 4x + 2, && 5!L_5(x) = -x^5 + 25x^4 - 200x^3 + 600x^2 - 600x + 120.
\end{aligned}$$

The functions $L_0(x)$, $L_1(x)$, $L_2(x)$ and $L_3(x)$ are plotted in figure 18.7.

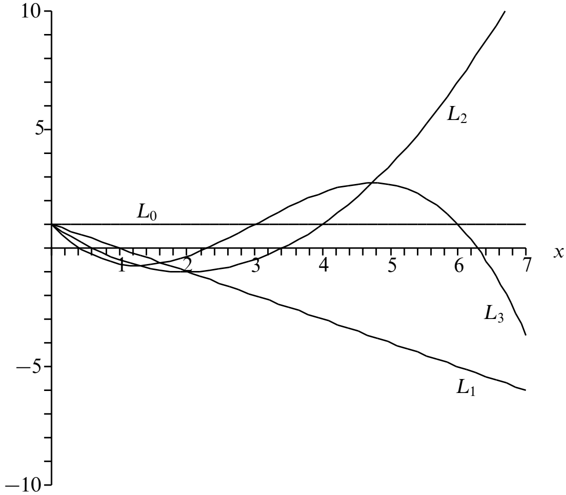

Figure 18.7 The first four Laguerre polynomials.

18.7.1 Properties of Laguerre polynomials

The Laguerre polynomials and functions derived from them are important in the analysis of the quantum mechanical behaviour of some physical systems. We therefore briefly outline their useful properties in this section.

Rodrigues' formula

The Laguerre polynomials can be expressed in terms of a Rodrigues' formula given by

$$L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}\left(x^n e^{-x}\right), \tag{18.112}$$

which may be proved straightforwardly by calculating the nth derivative explicitly using Leibnitz' theorem and comparing the result with (18.111). This is illustrated in the following example.

►*Prove that the expression (18.112) yields the nth Laguerre polynomial.*

Evaluating the nth derivative in (18.112) using Leibnitz' theorem, we find

$$\begin{aligned} L_n(x) &= \frac{e^x}{n!}\sum_{r=0}^{n} {}^nC_r \frac{d^r x^n}{dx^r}\frac{d^{n-r}e^{-x}}{dx^{n-r}} \\ &= \frac{e^x}{n!}\sum_{r=0}^{n} \frac{n!}{r!(n-r)!}\frac{n!}{(n-r)!}x^{n-r}(-1)^{n-r}e^{-x} \\ &= \sum_{r=0}^{n}(-1)^{n-r}\frac{n!}{r!(n-r)!(n-r)!}x^{n-r}. \end{aligned}$$

Relabelling the summation using the index $m = n - r$, we obtain

$$L_n(x) = \sum_{m=0}^{n}(-1)^m \frac{n!}{(m!)^2(n-m)!}x^m,$$

which is precisely the expression (18.111) for the nth Laguerre polynomial. ◄

Mutual orthogonality

In section 17.4, we noted that Laguerre's equation could be put into Sturm–Liouville form with $p = xe^{-x}$, $q = 0$, $\lambda = \nu$ and $\rho = e^{-x}$, and its natural interval is thus $[0, \infty]$. Since the Laguerre polynomials $L_n(x)$ are solutions of the equation and are regular at the end-points, they must be mutually orthogonal over this interval with respect to the weight function $\rho = e^{-x}$, i.e.

$$\int_0^\infty L_n(x)L_k(x)e^{-x}\,dx = 0 \qquad \text{if } n \neq k.$$

This result may also be proved directly using the Rodrigues' formula (18.112). Indeed, the normalisation, when $k = n$, is most easily found using this method.

►*Show that*

$$I \equiv \int_0^\infty L_n(x)L_n(x)e^{-x}\,dx = 1. \tag{18.113}$$

Using the Rodrigues' formula (18.112), we may write

$$I = \frac{1}{n!}\int_0^\infty L_n(x)\frac{d^n}{dx^n}(x^n e^{-x})\,dx = \frac{(-1)^n}{n!}\int_0^\infty \frac{d^n L_n}{dx^n}x^n e^{-x}\,dx,$$

where, in the second equality, we have integrated by parts n times and used the fact that the boundary terms all vanish. When d^nL_n/dx^n is evaluated using (18.111), only the derivative of the $m = n$ term survives and that has the value $[(-1)^n n!\,n!]/[(n!)^2\,0!] = (-1)^n$. Thus we have

$$I = \frac{1}{n!}\int_0^\infty x^n e^{-x}\,dx = 1,$$

where, in the second equality, we use the expression (18.153) defining the gamma function (see section 18.12). ◄

The above orthogonality and normalisation conditions allow us to expand any (reasonable) function in the interval $0 \leq x < \infty$ in a series of the form

$$f(x) = \sum_{n=0}^{\infty} a_n L_n(x),$$

in which the coefficients a_n are given by

$$a_n = \int_0^{\infty} f(x) L_n(x) e^{-x}\, dx.$$

We note that it is sometimes convenient to define the *orthonormal Laguerre functions* $\phi_n(x) = e^{-x/2} L_n(x)$, which may also be used to produce a series expansion of a function in the interval $0 \leq x < \infty$.

Generating function

The generating function for the Laguerre polynomials is given by

$$G(x,h) = \frac{e^{-xh/(1-h)}}{1-h} = \sum_{n=0}^{\infty} L_n(x) h^n. \tag{18.114}$$

We may prove this result by differentiating the generating function with respect to x and h, respectively, to obtain recurrence relations for the Laguerre polynomials, which may then be combined to show that the functions $L_n(x)$ in (18.114) do indeed satisfy Laguerre's equation (as discussed in the next subsection).

Recurrence relations

The Laguerre polynomials obey a number of useful recurrence relations. The three most important relations are as follows:

$$(n+1)L_{n+1}(x) = (2n+1-x)L_n(x) - nL_{n-1}(x), \tag{18.115}$$

$$L_{n-1}(x) = L'_{n-1}(x) - L'_n(x), \tag{18.116}$$

$$xL'_n(x) = nL_n(x) - nL_{n-1}(x). \tag{18.117}$$

The first two relations are easily derived from the generating function (18.114), and may be combined straightforwardly to yield the third result.

►*Derive the recurrence relations (18.115) and (18.116).*

Differentiating the generating function (18.114) with respect to h, we find

$$\frac{\partial G}{\partial h} = \frac{(1-x-h)e^{-xh/(1-h)}}{(1-h)^3} = \sum nL_n h^{n-1}.$$

Thus, we may write

$$(1-x-h)\sum L_n h^n = (1-h)^2 \sum nL_n h^{n-1},$$

and, on equating coefficients of h^n on each side, we obtain

$$(1-x)L_n - L_{n-1} = (n+1)L_{n+1} - 2nL_n + (n-1)L_{n-1},$$

which trivially rearranges to give the recurrence relation (18.115).

To obtain the recurrence relation (18.116), we begin by differentiating the generating function (18.114) with respect to x, which yields

$$\frac{\partial G}{\partial x} = -\frac{he^{-xh/(1-h)}}{(1-h)^2} = \sum L_n' h^n,$$

and thus we have

$$-h\sum L_n h^n = (1-h)\sum L_n' h^n.$$

Equating coefficients of h^n on each side then gives

$$-L_{n-1} = L_n' - L_{n-1}',$$

which immediately simplifies to give (18.116). ◄

18.8 Associated Laguerre functions

The associated Laguerre equation has the form

$$xy'' + (m+1-x)y' + ny = 0; \qquad (18.118)$$

it has a regular singularity at $x = 0$ and an essential singularity at $x = \infty$. We restrict our attention to the situation in which the parameters n and m are both non-negative integers, as is the case in nearly all physical problems. The associated Laguerre equation occurs most frequently in quantum-mechanical applications. Any solution of (18.118) is called an *associated Laguerre function.*

Solutions of (18.118) for non-negative integers n and m are given by the *associated Laguerre polynomials*

$$L_n^m(x) = (-1)^m \frac{d^m}{dx^m} L_{n+m}(x), \qquad (18.119)$$

where $L_n(x)$ are the ordinary Laguerre polynomials.[§]

► *Show that the functions $L_n^m(x)$ defined in (18.119) are solutions of (18.118).*

Since the Laguerre polynomials $L_n(x)$ are solutions of Laguerre's equation (18.107), we have

$$xL_{n+m}'' + (1-x)L_{n+m}' + (n+m)L_{n+m} = 0.$$

Differentiating this equation m times using Leibnitz' theorem and rearranging, we find

$$xL_{n+m}^{(m+2)} + (m+1-x)L_{n+m}^{(m+1)} + nL_{n+m}^{(m)} = 0.$$

On multiplying through by $(-1)^m$ and setting $L_n^m = (-1)^m L_{n+m}^{(m)}$, in accord with (18.119), we obtain

$$x(L_n^m)'' + (m+1-x)(L_n^m)' + nL_n^m = 0,$$

which shows that the functions L_n^m are indeed solutions of (18.118). ◄

[§] Note that some authors define the associated Laguerre polynomials as $\mathcal{L}_n^m(x) = (d^m/dx^m)L_n(x)$, which is thus related to our expression (18.119) by $L_n^m(x) = (-1)^m \mathcal{L}_{n+m}^m(x)$.

In particular, we note that $L_n^0(x) = L_n(x)$. As discussed in the previous section, $L_n(x)$ is a polynomial of order n and so it follows that $L_n^m(x)$ is also. The first few associated Laguerre polynomials are easily found using (18.119):

$$
\begin{aligned}
L_0^m(x) &= 1, \\
L_1^m(x) &= -x + m + 1, \\
2!L_2^m(x) &= x^2 - 2(m+2)x + (m+1)(m+2), \\
3!L_3^m(x) &= -x^3 + 3(m+3)x^2 - 3(m+2)(m+3)x + (m+1)(m+2)(m+3).
\end{aligned}
$$

Indeed, in the general case, one may show straightforwardly, from the definition (18.119) and the expression (18.111) for the ordinary Laguerre polynomials, that

$$L_n^m(x) = \sum_{k=0}^{n} (-1)^k \frac{(n+m)!}{k!(n-k)!(k+m)!} x^k. \qquad (18.120)$$

18.8.1 Properties of associated Laguerre polynomials

The properties of the associated Laguerre polynomials follow directly from those of the ordinary Laguerre polynomials through the definition (18.119). We shall therefore only briefly outline the most useful results here.

Rodrigues' formula

A Rodrigues' formula for the associated Laguerre polynomials is given by

$$L_n^m(x) = \frac{e^x x^{-m}}{n!} \frac{d^n}{dx^n}(x^{n+m} e^{-x}). \qquad (18.121)$$

It can be proved by evaluating the nth derivative using Leibnitz' theorem (see exercise 18.7).

Mutual orthogonality

In section 17.4, we noted that the associated Laguerre equation could be transformed into a Sturm–Liouville one with $p = x^{m+1}e^{-x}$, $q = 0$, $\lambda = n$ and $\rho = x^m e^{-x}$, and its natural interval is thus $[0, \infty]$. Since the associated Laguerre polynomials $L_n^m(x)$ are solutions of the equation and are regular at the end-points, those with the same m but differing values of the eigenvalue $\lambda = n$ must be mutually orthogonal over this interval with respect to the weight function $\rho = x^m e^{-x}$, i.e.

$$\int_0^\infty L_n^m(x) L_k^m(x) x^m e^{-x}\, dx = 0 \qquad \text{if } n \neq k.$$

This result may also be proved directly using the Rodrigues' formula (18.121), as may the normalisation condition when $k = n$.

►*Show that*

$$I \equiv \int_0^\infty L_n^m(x) L_n^m(x) x^m e^{-x}\, dx = \frac{(n+m)!}{n!}. \qquad (18.122)$$

Using the Rodrigues' formula (18.121), we may write

$$I = \frac{1}{n!}\int_0^\infty L_n^m(x)\frac{d^n}{dx^n}(x^{n+m}e^{-x})\, dx = \frac{(-1)^n}{n!}\int_0^\infty \frac{d^n L_n^m}{dx^n} x^{n+m} e^{-x}\, dx,$$

where, in the second equality, we have integrated by parts n times and used the fact that the boundary terms all vanish. From (18.120) we see that $d^n L_n^m/dx^n = (-1)^n$. Thus we have

$$I = \frac{1}{n!}\int_0^\infty x^{n+m} e^{-x}\, dx = \frac{(n+m)!}{n!},$$

where, in the second equality, we use the expression (18.153) defining the gamma function (see section 18.12). ◄

The above orthogonality and normalisation conditions allow us to expand any (reasonable) function in the interval $0 \le x < \infty$ in a series of the form

$$f(x) = \sum_{n=0}^{\infty} a_n L_n^m(x),$$

in which the coefficients a_n are given by

$$a_n = \frac{n!}{(n+m)!}\int_0^\infty f(x) L_n^m(x) x^m e^{-x}\, dx.$$

We note that it is sometimes convenient to define the *orthogonal associated Laguerre functions* $\phi_n^m(x) = x^{m/2}e^{-x/2}L_n^m(x)$, which may also be used to produce a series expansion of a function in the interval $0 \le x < \infty$.

Generating function

The generating function for the associated Laguerre polynomials is given by

$$G(x,h) = \frac{e^{-xh/(1-h)}}{(1-h)^{m+1}} = \sum_{n=0}^{\infty} L_n^m(x) h^n. \qquad (18.123)$$

This can be obtained by differentiating the generating function (18.114) for the ordinary Laguerre polynomials m times with respect to x, and using (18.119).

►*Use the generating function (18.123) to obtain an expression for* $L_n^m(0)$.

From (18.123), we have

$$\begin{aligned}\sum_{n=0}^{\infty} L_n^m(0) h^n &= \frac{1}{(1-h)^{m+1}} \\ &= 1 + (m+1)h + \frac{(m+1)(m+2)}{2!}h^2 + \cdots + \frac{(m+1)(m+2)\cdots(m+n)}{n!}h^n + \cdots,\end{aligned}$$

where, in the second equality, we have expanded the RHS using the binomial theorem. On equating coefficients of h^n, we immediately obtain

$$L_n^m(0) = \frac{(n+m)!}{n!m!}. \blacktriangleleft$$

Recurrence relations

The various recurrence relations satisfied by the associated Laguerre polynomials may be derived by differentiating the generating function (18.123) with respect to either or both of x and h, or by differentiating with respect to x the recurrence relations obeyed by the ordinary Laguerre polynomials, discussed in section 18.7.1. Of the many recurrence relations satisfied by the associated Laguerre polynomials, two of the most useful are as follows:

$$(n+1)L_{n+1}^m(x) = (2n+m+1-x)L_n^m(x) - (n+m)L_{n-1}^m(x), \qquad (18.124)$$

$$x(L_n^m)'(x) = nL_n^m(x) - (n+m)L_{n-1}^m(x). \qquad (18.125)$$

For proofs of these relations the reader is referred to exercise 18.7.

18.9 Hermite functions

Hermite's equation has the form

$$y'' - 2xy' + 2\nu y = 0, \qquad (18.126)$$

and has an essential singularity at $x = \infty$. The parameter ν is a given real number, although it nearly always takes an integer value in physical applications. The Hermite equation appears in the description of the wavefunction of the harmonic oscillator. Any solution of (18.126) is called a *Hermite function.*

Since $x = 0$ is an ordinary point of the equation, we may find two linearly independent solutions in the form of a power series (see section 16.2):

$$y(x) = \sum_{m=0}^{\infty} a_m x^m. \qquad (18.127)$$

Substituting this series into (18.107) yields

$$\sum_{m=0}^{\infty} \left[(m+1)(m+2)a_{m+2} + 2(\nu - m)a_m\right] x^m = 0.$$

Demanding that the coefficient of each power of x vanishes, we obtain the recurrence relation

$$a_{m+2} = -\frac{2(\nu - m)}{(m+1)(m+2)} a_m.$$

As mentioned above, in nearly all physical applications, the parameter ν takes integer values. Therefore, if $\nu = n$, where n is a non-negative integer, we see that

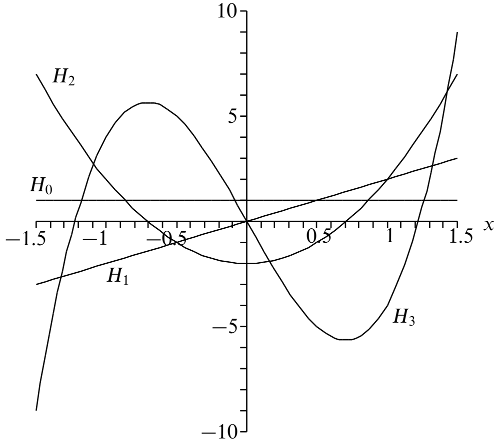

Figure 18.8 The first four Hermite polynomials.

$a_{n+2} = a_{n+4} = \cdots = 0$, and so one solution of Hermite's equation is a polynomial of order n. For even n, it is conventional to choose $a_0 = (-1)^{n/2} n!/(n/2)!$, whereas for odd n one takes $a_1 = (-1)^{(n-1)/2} 2n!/[\frac{1}{2}(n-1)]!$. These choices allow a general solution to be written as

$$H_n(x) = (2x)^n - n(n-1)(2x)^{n-1} + \frac{n(n-1)(n-2)(n-3)}{2!}(2x)^{n-4} - \cdots \tag{18.128}$$

$$= \sum_{m=0}^{[n/2]} (-1)^m \frac{n!}{m!(n-2m)!}(2x)^{n-2m}, \tag{18.129}$$

where $H_n(x)$ is called the nth *Hermite polynomial* and the notation $[n/2]$ denotes the integer part of $n/2$. We note in particular that $H_n(-x) = (-1)^n H_n(x)$. The first few Hermite polynomials are given by

$$H_0(x) = 1, \qquad H_3(x) = 8x^2 - 12x,$$
$$H_1(x) = 2x, \qquad H_4(x) = 16x^4 - 48x^2 + 12,$$
$$H_2(x) = 4x^2 - 2, \qquad H_5(x) = 32x^5 - 160x^3 + 120x.$$

The functions $H_0(x)$, $H_1(x)$, $H_2(x)$ and $H_3(x)$ are plotted in figure 18.8.

18.9.1 Properties of Hermite polynomials

The Hermite polynomials and functions derived from them are important in the analysis of the quantum mechanical behaviour of some physical systems. We therefore briefly outline their useful properties in this section.

Rodrigues' formula

The Rodrigues' formula for the Hermite polynomials is given by

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}(e^{-x^2}). \tag{18.130}$$

This can be proved using Leibnitz' theorem.

►*Prove the Rodrigues' formula (18.130) for the Hermite polynomials.*

Letting $u = e^{-x^2}$ and differentiating with respect to x, we quickly find that

$$u' + 2xu = 0.$$

Differentiating this equation $n+1$ times using Leibnitz' theorem then gives

$$u^{(n+2)} + 2xu^{(n+1)} + 2(n+1)u^{(n)} = 0,$$

which, on introducing the new variable $v = (-1)^n u^{(n)}$, reduces to

$$v'' + 2xv' + 2(n+1)v = 0. \tag{18.131}$$

Now letting $y = e^{x^2}v$, we may write the derivatives of v as

$$v' = e^{-x^2}(y' - 2xy),$$
$$v'' = e^{-x^2}(y'' - 4xy' + 4x^2y - 2y).$$

Substituting these expressions into (18.131), and dividing through by e^{-x^2}, finally yields Hermite's equation,

$$y'' - 2xy + 2ny = 0,$$

thus demonstrating that $y = (-1)^n e^{x^2} d^n(e^{-x^2})/dx^n$ is indeed a solution. Moreover, since this solution is clearly a polynomial of order n, it must be some multiple of $H_n(x)$. The normalisation is easily checked by noting that, from (18.130), the highest-order term is $(2x)^n$, which agrees with the expression (18.128). ◄

Mutual orthogonality

We saw in section 17.4 that Hermite's equation could be cast in Sturm–Liouville form with $p = e^{-x^2}$, $q = 0$, $\lambda = 2n$ and $\rho = e^{-x^2}$, and its natural interval is thus $[-\infty, \infty]$. Since the Hermite polynomials $H_n(x)$ are solutions of the equation and are regular at the end-points, they must be mutually orthogonal over this interval with respect to the weight function $\rho = e^{-x^2}$, i.e.

$$\int_{-\infty}^{\infty} H_n(x)H_k(x)e^{-x^2}\,dx = 0 \qquad \text{if } n \neq k.$$

This result may also be proved directly using the Rodrigues' formula (18.130). Indeed, the normalisation, when $k = n$, is most easily found in this way.

►*Show that*

$$I \equiv \int_{-\infty}^{\infty} H_n(x)H_n(x)e^{-x^2}\,dx = 2^n n!\sqrt{\pi}. \tag{18.132}$$

Using the Rodrigues' formula (18.130), we may write

$$I = (-1)^n \int_0^{\infty} H_n(x)\frac{d^n}{dx^n}(e^{-x^2})\,dx = \int_{-\infty}^{\infty} \frac{d^n H_n}{dx^n}\,e^{-x^2}\,dx,$$

where, in the second equality, we have integrated by parts n times and used the fact that the boundary terms all vanish. From (18.128) we see that $d^n H_n/dx^n = 2^n n!$. Thus we have

$$I = 2^n n! \int_{-\infty}^{\infty} e^{-x^2}\,dx = 2^n n!\sqrt{\pi},$$

where, in the second equality, we use the standard result for the area under a Gaussian (see section 6.4.2). ◄

The above orthogonality and normalisation conditions allow any (reasonable) function in the interval $-\infty \leq x < \infty$ to be expanded in a series of the form

$$f(x) = \sum_{n=0}^{\infty} a_n H_n(x),$$

in which the coefficients a_n are given by

$$a_n = \frac{1}{2^n n!\sqrt{\pi}} \int_{-\infty}^{\infty} f(x)H_n(x)e^{-x^2}\,dx.$$

We note that it is sometimes convenient to define the *orthogonal Hermite functions* $\phi_n(x) = e^{-x^2/2}H_n(x)$; they also may be used to produce a series expansion of a function in the interval $-\infty \leq x < \infty$. Indeed, $\phi_n(x)$ is proportional to the wavefunction of a particle in the nth energy level of a quantum harmonic oscillator.

Generating function

The generating function equation for the Hermite polynomials reads

$$G(x,h) = e^{2hx-h^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!}h^n, \tag{18.133}$$

a result that may be proved using the Rodrigues' formula (18.130).

►*Show that the functions $H_n(x)$ in (18.133) are the Hermite polynomials.*

It is often more convenient to write the generating function (18.133) as

$$G(x,h) = e^{x^2}e^{-(x-h)^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!}h^n.$$

Differentiating this form k times with respect to h gives

$$\sum_{n=k}^{\infty} \frac{H_n}{(n-k)!} h^{n-k} = \frac{\partial^k G}{\partial h^k} = e^{x^2} \frac{\partial^k}{\partial h^k} e^{-(x-h)^2} = (-1)^k e^{x^2} \frac{\partial^k}{\partial x^k} e^{-(x-h)^2}.$$

Relabelling the summation on the LHS using the new index $m = n - k$, we obtain

$$\sum_{m=0}^{\infty} \frac{H_{m+k}}{m!} h^m = (-1)^k e^{x^2} \frac{\partial^k}{\partial x^k} e^{-(x-h)^2}.$$

Setting $h = 0$ in this equation, we find

$$H_k(x) = (-1)^k e^{x^2} \frac{d^k}{dx^k} (e^{-x^2}),$$

which is the Rodrigues' formula (18.130) for the Hermite polynomials. ◄

The generating function (18.133) is also useful for determining special values of the Hermite polynomials. In particular, it is straightforward to show that $H_{2n}(0) = (-1)^n (2n)!/n!$ and $H_{2n+1}(0) = 0$.

Recurrence relations

The two most useful recurrence relations satisfied by the Hermite polynomials are given by

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \tag{18.134}$$

$$H_n'(x) = 2nH_{n-1}(x). \tag{18.135}$$

The first relation provides a simple iterative way of evaluating the nth Hermite polynomials at some point $x = x_0$, given the values of $H_0(x)$ and $H_1(x)$ at that point. For proofs of these recurrence relations, see exercise 18.5.

18.10 Hypergeometric functions

The hypergeometric equation has the form

$$x(1-x)y'' + [c - (a + b + 1)x]y' - aby = 0, \tag{18.136}$$

and has three regular singular points, at $x = 0, 1, \infty$, but no essential singularities. The parameters a, b and c are given real numbers.

In our discussions of Legendre functions, associated Legendre functions and Chebyshev functions in sections 18.1, 18.2 and 18.4, respectively, it was noted that in each case the corresponding second-order differential equation had three regular singular points, at $x = -1, 1, \infty$, and no essential singularities. The hypergeometric equation can, in fact, be considered as the 'canonical form' for second-order differential equations with this number of singularities. It may be shown[§] that,

[§] See, for example, J. Mathews and R. L. Walker, *Mathematical Methods of Physics*, 2nd edn (Reading MA: Addision–Wesley, 1971).

by making appropriate changes of the independent and dependent variables, any second-order differential equation with three regular singularities and an ordinary point at infinity can be transformed into the hypergeometric equation (18.136) with the singularities at $= -1$, 1 and ∞. As we discuss below, this allows Legendre functions, associated Legendre functions and Chebyshev functions, for example, to be written as particular cases of *hypergeometric functions*, which are the solutions to (18.136).

Since the point $x = 0$ is a regular singularity of (18.136), we may find at least one solution in the form of a Frobenius series (see section 16.3):

$$y(x) = \sum_{n=0}^{\infty} a_n x^{n+\sigma}. \tag{18.137}$$

Substituting this series into (18.136) and dividing through by $x^{\sigma-1}$, we obtain

$$\sum_{n=0}^{\infty} \{(1-x)(n+\sigma)(n+\sigma-1) + [c-(a+b+1)x](n+\sigma) - abx\}\, a_n x^n = 0. \tag{18.138}$$

Setting $x = 0$, so that only the $n = 0$ term remains, we obtain the indicial equation $\sigma(\sigma-1) + c\sigma = 0$, which has the roots $\sigma = 0$ and $\sigma = 1 - c$. Thus, provided c is not an integer, one can obtain two linearly independent solutions of the hypergeometric equation in the form (18.137).

For $\sigma = 0$ the corresponding solution is a simple power series. Substituting $\sigma = 0$ into (18.138) and demanding that the coefficient of x^n vanishes, we find the recurrence relation

$$n[(n-1)+c]a_n - [(n-1)(a+b+n-1)+ab]a_{n-1} = 0, \tag{18.139}$$

which, on simplifying and replacing n by $n+1$, yields the recurrence relation

$$a_{n+1} = \frac{(a+n)(b+n)}{(n+1)(c+n)} a_n. \tag{18.140}$$

It is conventional to make the simple choice $a_0 = 1$. Thus, provided c is not a negative integer or zero, we may write the solution as follows:

$$F(a,b,c;x) = 1 + \frac{ab}{c}\frac{x}{1!} + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{x^2}{2!} + \cdots \tag{18.141}$$

$$= \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)}\frac{x^n}{n!}, \tag{18.142}$$

where $F(a,b,c;x)$ is known as the *hypergeometric function* or *hypergeometric series*, and in the second equality we have used the property (18.154) of the gamma function.[§] It is straightforward to show that the hypergeometric series converges in the range $|x| < 1$. It also converges at $x = 1$ if $c > a + b$ and at $x = -1$ if $c > a + b - 1$. We also note that $F(a, b, c; x)$ is symmetric in the parameters a and b, i.e. $F(a, b, c; x) = F(b, a, c; x)$.

The hypergeometric function $y(x) = F(a, b, c; x)$ is clearly not the general solution to the hypergeometric equation (18.136), since we must also consider the second root of the indicial equation. Substituting $\sigma = 1 - c$ into (18.138) and demanding that the coefficient of x^n vanishes, we find that we must have

$$n(n + 1 - c)a_n - [(n - c)(a + b + n - c) + ab]a_{n-1} = 0,$$

which, on comparing with (18.139) and replacing n by $n+1$, yields the recurrence relation

$$a_{n+1} = \frac{(a - c + 1 + n)(b - c + 1 + n)}{(n + 1)(2 - c + n)} a_n.$$

We see that this recurrence relation has the same form as (18.140) if one makes the replacements $a \to a - c + 1$, $b \to b - c + 1$ and $c \to 2 - c$. Thus, provided c, $a-b$ and $c-a-b$ are all non-integers, the general solution to the hypergeometric equation, valid for $|x| < 1$, may be written as

$$y(x) = AF(a, b, c; x) + Bx^{1-c}F(a - c + 1, b - c + 1, 2 - c; x), \tag{18.143}$$

where A and B are arbitrary constants to be fixed by the boundary conditions on the solution. If the solution is to be regular at $x = 0$, one requires $B = 0$.

18.10.1 Properties of hypergeometric functions

Since the hypergeometric equation is so general in nature, it is not feasible to present a comprehensive account of the hypergeometric functions. Nevertheless, we outline here some of their most important properties.

Special cases

As mentioned above, the general nature of the hypergeometric equation allows us to write a large number of elementary functions in terms of the hypergeometric functions $F(a, b, c; x)$. Such identifications can be made from the series expansion (18.142) directly, or by transformation of the hypergeometric equation into a more familiar equation, the solutions to which are already known. Some particular examples of well known special cases of the hypergeometric function are as follows:

[§] We note that it is also common to denote the hypergeometric function by ${}_2F_1(a, b, c; x)$. This slightly odd-looking notation is meant to signify that, in the coefficient of each power of x, there are two parameters (a and b) in the numerator and one parameter (c) in the denominator.

$$F(a,b,b;x) = (1-x)^{-a}, \qquad F(\tfrac{1}{2},\tfrac{1}{2},\tfrac{3}{2};x^2) = x^{-1}\sin^{-1}x,$$

$$F(1,1,2;-x) = x^{-1}\ln(1+x), \qquad F(\tfrac{1}{2},1,\tfrac{3}{2};-x^2) = x^{-1}\tan^{-1}x,$$

$$\lim_{m\to\infty} F(1,m,1;x/m) = e^x, \qquad F(\tfrac{1}{2},1,\tfrac{3}{2};x^2) = \tfrac{1}{2}x^{-1}\ln[(1+x)/(1-x)],$$

$$F(\tfrac{1}{2},-\tfrac{1}{2},\tfrac{1}{2};\sin^2 x) = \cos x, \qquad F(m+1,-m,1;(1-x)/2) = P_m(x),$$

$$F(\tfrac{1}{2},p,p;\sin^2 x) = \sec x, \qquad F(m,-m,\tfrac{1}{2};(1-x)/2) = T_m(x),$$

where m is an integer, $P_m(x)$ is the mth Legendre polynomial and $T_m(x)$ is the mth Chebyshev polynomial of the first kind. Some of these results are proved in exercise 18.11.

►*Show that* $F(m,-m,\frac{1}{2};(1-x)/2) = T_m(x)$.

Let us prove this result by transforming the hypergeometric equation. The form of the result suggests that we should make the substitution $x = (1-z)/2$ into (18.136), in which case $d/dx = -2d/dz$. Thus, letting $u(z) = y(x)$ and setting $a = m$, $b = -m$ and $c = 1/2$, (18.136) becomes

$$\frac{(1-z)}{2}\frac{(1+z)}{2}(-2)^2\frac{d^2u}{dz^2} + \left[\tfrac{1}{2} - (m-m+1)\frac{1-z}{2}\right](-2)\frac{du}{dz} - (m)(-m)u = 0.$$

On simplifying, we obtain

$$(1-z^2)\frac{d^2u}{dz^2} - z\frac{du}{dz} + m^2u = 0,$$

which has the form of Chebyshev's equation, (18.54). This equation has $u(z) = T_m(z)$ as its power series solution, and so $F(m,-m,\frac{1}{2};(1-z)/2)$ and $T_m(z)$ are equal to within a normalisation factor. On comparing the expressions (18.141) and (18.56) at $x = 0$, i.e. at $z = 1$, we see that they both have value 1. Hence, the normalisations already agree and we obtain the required result. ◄

Integral representation

One of the most useful representations for the hypergeometric functions is in terms of an integral, which may be derived using the properties of the gamma and beta functions discussed in section 18.12. The integral representation reads

$$F(a,b,c;x) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-tx)^{-a}\,dt, \tag{18.144}$$

and requires $c > b > 0$ for the integral to converge.

►*Prove the result (18.144).*

From the series expansion (18.142), we have

$$\begin{aligned} F(a,b,c;x) &= \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)}\sum_{n=0}^{\infty}\frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)}\frac{x^n}{n!} \\ &= \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)\Gamma(c-b)}\sum_{n=0}^{\infty}\Gamma(a+n)B(b+n,c-b)\frac{x^n}{n!}, \end{aligned}$$

where in the second equality we have used the expression (18.165) relating the gamma and beta functions. Using the definition (18.162) of the beta function, we then find

$$\begin{aligned} F(a,b,c;x) &= \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)\Gamma(c-b)} \sum_{n=0}^{\infty} \Gamma(a+n)\frac{x^n}{n!} \int_0^1 t^{b+n-1}(1-t)^{c-b-1}\,dt \\ &= \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 dt\, t^{b-1}(1-t)^{c-b-1} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(a)}\frac{(tx)^n}{n!}, \end{aligned}$$

where in the second equality we have rearranged the expression and reversed the order of integration and summation. Finally, one recognises the sum over n as being equal to $(1-tx)^{-a}$, and so we obtain the final result (18.144). ◀

The integral representation may be used to prove a wide variety of properties of the hypergeometric functions. As a simple example, on setting $x = 1$ in (18.144), and using properties of the beta function discussed in section 18.12.2, one quickly finds that, provided c is not a negative integer or zero and $c > a + b$,

$$F(a,b,c;1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}.$$

Relationships between hypergeometric functions

There exist a great many relationships between hypergeometric functions with different arguments. These are most easily derived by making use of the integral representation (18.144) or the series form (18.141). It is not feasible to list all the relationships here, so we simply note two useful examples, which read

$$F(a,b,c;x) = (1-x)^{c-a-b}F(c-a,c-b,c;x), \tag{18.145}$$

$$F'(a,b,c;x) = \frac{ab}{c}F(a+1,b+1,c+1;x), \tag{18.146}$$

where the prime in the second relation denotes d/dx. The first result follows straightforwardly from the integral representation using the substitution $t = (1-u)/(1-ux)$, whereas the second result may be proved more easily from the series expansion.

In addition to the above results, one may also derive relationships between $F(a,b,c;x)$ and any two of the six 'contiguous functions' $F(a\pm 1,b,c;x)$, $F(a,b\pm 1,c;x)$ and $F(a,b,c\pm 1;x)$. These 'contiguous relations' serve as the recurrence relations for the hypergeometric functions. An example of such a relationship is

$$(c-a)F(a-1,b,c;x) + (2a-c-ax+bx)F(a,b,c;x) + a(x-1)F(a+1,b,c;x) = 0.$$

Repeated application of such relationships allows one to express $F(a+l,b+m,c+n;x)$, where l,m,n are integers (with $c+n$ not equalling a negative integer or zero), as a linear combination of $F(a,b,c;x)$ and one of its contiguous functions.

18.11 Confluent hypergeometric functions

The confluent hypergeometric equation has the form

$$xy'' + (c - x)y' - ay = 0; \tag{18.147}$$

it has a regular singularity at $x = 0$ and an essential singularity at $x = \infty$. This equation can be obtained by merging two of the singularities of the ordinary hypergeometric equation (18.136). The parameters a and c are given real numbers.

►*Show that setting $x = z/b$ in the hypergeometric equation, and letting $b \to \infty$, yields the confluent hypergeometric equation.*

Substituting $x = z/b$ into (18.136), with $d/dx = b\,d/dz$, and letting $u(z) = y(x)$, we obtain

$$bz\left(1 - \frac{z}{b}\right)\frac{d^2u}{dz^2} + [bc - (a + b + 1)z]\frac{du}{dz} - abu = 0,$$

which clearly has regular singular points at $z = 0$, b and ∞. If we now merge the last two singularities by letting $b \to \infty$, we obtain

$$zu'' + (c - z)u' - au = 0,$$

where the primes denote d/dz. Hence $u(z)$ must satisfy the confluent hypergeometric equation. ◄

In our discussion of Bessel, Laguerre and associated Laguerre functions, it was noted that the corresponding second-order differential equation in each case had a single regular singular point at $x = 0$ and an essential singularity at $x = \infty$. From table 16.1, we see that this is also true for the confluent hypergeometric equation. Indeed, this equation can be considered as the 'canonical form' for second-order differential equations with this pattern of singularities. Consequently, as we mention below, the Bessel, Laguerre and associated Laguerre functions can all be written in terms of the *confluent hypergeometric functions*, which are the solutions of (18.147).

The solutions of the confluent hypergeometric equation are obtained from those of the ordinary hypergeometric equation by again letting $x \to x/b$ and carrying out the limiting process $b \to \infty$. Thus, from (18.141) and (18.143), two linearly independent solutions of (18.147) are (when c is not an integer)

$$y_1(x) = 1 + \frac{a}{c}\frac{x}{1!} + \frac{a(a+1)}{c(c+1)}\frac{z^2}{2!} + \cdots \equiv M(a, c; x), \tag{18.148}$$

$$y_2(x) = x^{1-c}M(a - c + 1, 2 - c; x), \tag{18.149}$$

where $M(a, c; x)$ is called the *confluent hypergeometric function* (or *Kummer function*).[§] It is worth noting, however, that $y_1(x)$ is singular when $c = 0, -1, -2, \ldots$ and $y_2(x)$ is singular when $c = 2, 3, 4, \ldots$. Thus, it is conventional to take the

[§] We note that an alternative notation for the confluent hypergeometric function is ${}_1F_1(a, c; x)$.

second solution to (18.147) as a linear combination of (18.148) and (18.149) given by

$$U(a, c; x) \equiv \frac{\pi}{\sin \pi c}\left[\frac{M(a, c; x)}{\Gamma(a-c+1)\Gamma(c)} - x^{1-c}\frac{M(a-c+1, 2-c; x)}{\Gamma(a)\Gamma(2-c)}\right].$$

This has a well behaved limit as c approaches an integer.

18.11.1 Properties of confluent hypergeometric functions

The properties of confluent hypergeometric functions can be derived from those of ordinary hypergeometric functions by letting $x \to x/b$ and taking the limit $b \to \infty$, in the same way as both the equation and its solution were derived. A general procedure of this sort is called a *confluence* process.

Special cases

The general nature of the confluent hypergeometric equation allows one to write a large number of elementary functions in terms of the confluent hypergeometric functions $M(a, c; x)$. Once again, such identifications can be made from the series expansion (18.148) directly, or by transformation of the confluent hypergeometric equation into a more familiar equation for which the solutions are already known. Some particular examples of well known special cases of the confluent hypergeometric function are as follows:

$$M(a, a; x) = e^x, \qquad M(1, 2; 2x) = \frac{e^x \sinh x}{x},$$

$$M(-n, 1; x) = L_n(x), \qquad M(-n, m+1; x) = \frac{n!m!}{(n+m)!}L_n^m(x),$$

$$M(-n, \tfrac{1}{2}; x^2) = \frac{(-1)^n n!}{(2n)!}H_{2n}(x), \qquad M(-n, \tfrac{3}{2}; x^2), = \frac{(-1)^n n!}{2(2n+1)!}\frac{H_{2n+1}(x)}{x},$$

$$M(\nu + \tfrac{1}{2}, 2\nu + 1; 2ix) = \nu!e^{ix}(\frac{x}{2})^{-\nu}J_\nu(x), \quad M(\tfrac{1}{2}, \tfrac{3}{2}; -x^2) = \frac{\sqrt{\pi}}{2x}\mathrm{erf}(x),$$

where n and m are integers, $L_n^m(x)$ is an associated Legendre polynomial, $H_n(x)$ is a Hermite polynomial, $J_\nu(x)$ is a Bessel function and $\mathrm{erf}(x)$ is the error function discussed in section 18.12.4.

Integral representation

Using the integral representation (18.144) of the ordinary hypergeometric function, exchanging a and b and carrying out the process of confluence gives

$$M(a, c, x) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)}\int_0^1 e^{tx}t^{a-1}(1-t)^{c-a-1}\,dt, \tag{18.150}$$

which converges provided $c > a > 0$.

►*Prove the result (18.150).*

Since $F(a, b, c; x)$ is unchanged by swapping a and b, we may write its integral representation (18.144) as

$$F(a, b, c; x) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 t^{a-1}(1-t)^{c-a-1}(1-tx)^{-b}\, dt.$$

Setting $x = z/b$ and taking the limit $b \to \infty$, we obtain

$$M(a, c; z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 t^{a-1}(1-t)^{c-a-1} \lim_{b\to\infty} \left(1 - \frac{tz}{b}\right)^{-b} dt.$$

Since the limit is equal to e^{tz}, we obtain result (18.150). ◄

Relationships between confluent hypergeometric functions

A large number of relationships exist between confluent hypergeometric functions with different arguments. These are straightforwardly derived using the integral representation (18.150) or the series form (18.148). Here, we simply note two useful examples, which read

$$M(a, c; x) = e^x M(c-a, c; -x), \tag{18.151}$$
$$M'(a, c; x) = \frac{a}{c} M(a+1, c+1; x), \tag{18.152}$$

where the prime in the second relation denotes d/dx. The first result follows straightforwardly from the integral representation, and the second result may be proved from the series expansion (see exercise 18.19).

In an analogous manner to that used for the ordinary hypergeometric functions, one may also derive relationships between $M(a, c; x)$ and any two of the four 'contiguous functions' $M(a \pm 1, c; x)$ and $M(a, c \pm 1; x)$. These serve as the recurrence relations for the confluent hypergeometric functions. An example of such a relationship is

$$(c-a)M(a-1, c; x) + (2a - c + x)M(a, c; x) - aM(a+1, c; x) = 0.$$

18.12 The gamma function and related functions

Many times in this chapter, and often throughout the rest of the book, we have made mention of the gamma function and related functions such as the beta and error functions. Although not derived as the solutions of important second-order ODEs, these convenient functions appear in a number of contexts, and so here we gather together some of their properties. This final section should be regarded merely as a reference containing some useful relations obeyed by these functions; a minimum of formal proofs is given.

18.12.1 The gamma function

The *gamma function* $\Gamma(n)$ is defined by

$$\Gamma(n) = \int_0^\infty x^{n-1} e^{-x}\, dx, \tag{18.153}$$

which converges for $n > 0$, where in general n is a real number. Replacing n by $n+1$ in (18.153) and integrating the RHS by parts, we find

$$\begin{aligned}\Gamma(n+1) &= \int_0^\infty x^n e^{-x}\, dx \\ &= \left[-x^n e^{-x}\right]_0^\infty + \int_0^\infty n x^{n-1} e^{-x}\, dx \\ &= n \int_0^\infty x^{n-1} e^{-x}\, dx,\end{aligned}$$

from which we obtain the important result

$$\Gamma(n+1) = n\Gamma(n). \tag{18.154}$$

From (18.153), we see that $\Gamma(1) = 1$, and so, if n is a positive integer,

$$\Gamma(n+1) = n!. \tag{18.155}$$

In fact, equation (18.155) serves as a definition of the factorial function even for non-integer n. For negative n the factorial function is defined by

$$n! = \frac{(n+m)!}{(n+m)(n+m-1)\cdots(n+1)}, \tag{18.156}$$

where m is any positive integer that makes $n+m > 0$. Different choices of m ($> -n$) do not lead to different values for $n!$. A plot of the gamma function is given in figure 18.9, where it can be seen that the function is infinite for negative integer values of n, in accordance with (18.156). For an extension of the factorial function to complex arguments, see exercise 18.15.

By letting $x = y^2$ in (18.153), we immediately obtain another useful representation of the gamma function given by

$$\Gamma(n) = 2\int_0^\infty y^{2n-1} e^{-y^2}\, dy. \tag{18.157}$$

Setting $n = \frac{1}{2}$ we find the result

$$\Gamma\left(\tfrac{1}{2}\right) = 2\int_0^\infty e^{-y^2}\, dy = \int_{-\infty}^\infty e^{-y^2}\, dy = \sqrt{\pi},$$

where have used the standard integral discussed in section 6.4.2. From this result, $\Gamma(n)$ for half-integral n can be found using (18.154). Some immediately derivable factorial values of half integers are

$$\left(-\tfrac{3}{2}\right)! = -2\sqrt{\pi}, \quad \left(-\tfrac{1}{2}\right)! = \sqrt{\pi}, \quad \left(\tfrac{1}{2}\right)! = \tfrac{1}{2}\sqrt{\pi}, \quad \left(\tfrac{3}{2}\right)! = \tfrac{3}{4}\sqrt{\pi}.$$

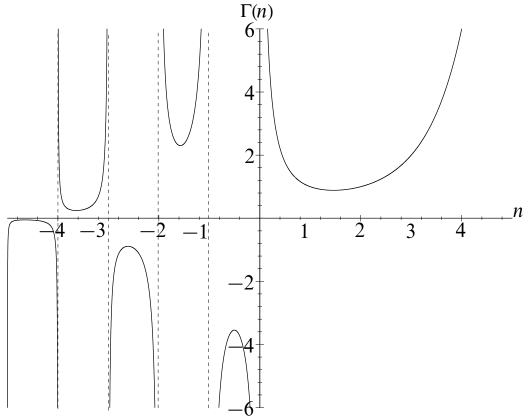

Figure 18.9 The gamma function $\Gamma(n)$.

Moreover, it may be shown for non-integral n that the gamma function satisfies the important identity

$$\Gamma(n)\Gamma(1-n) = \frac{\pi}{\sin n\pi}. \tag{18.158}$$

This is proved for a restricted range of n in the next section, once the beta function has been introduced.

It can also be shown that the gamma function is given by

$$\Gamma(n+1) = \sqrt{2\pi n}\; n^n e^{-n}\left(1 + \frac{1}{12n} + \frac{1}{288n^2} - \frac{139}{51\,840n^3} + \ldots\right) = n!, \tag{18.159}$$

which is known as *Stirling's asymptotic series*. For large n the first term dominates, and so

$$n! \approx \sqrt{2\pi n}\; n^n e^{-n}; \tag{18.160}$$

this is known as *Stirling's approximation*. This approximation is particularly useful in statistical thermodynamics, when arrangements of a large number of particles are to be considered.

►*Prove Stirling's approximation* $n! \approx \sqrt{2\pi n}\; n^n e^{-n}$ *for large n.*

From (18.153), the extended definition of the factorial function (which is valid for $n > -1$) is given by

$$n! = \int_0^\infty x^n e^{-x}\,dx = \int_0^\infty e^{n\ln x - x}\,dx. \tag{18.161}$$

If we let $x = n + y$, then

$$\begin{aligned}\ln x &= \ln n + \ln\left(1 + \frac{y}{n}\right)\\ &= \ln n + \frac{y}{n} - \frac{y^2}{2n^2} + \frac{y^3}{3n^3} - \cdots.\end{aligned}$$

Substituting this result into (18.161), we obtain

$$n! = \int_{-n}^{\infty} \exp\left[n\left(\ln n + \frac{y}{n} - \frac{y^2}{2n^2} + \cdots\right) - n - y\right] dy.$$

Thus, when n is sufficiently large, we may approximate $n!$ by

$$n! \approx e^{n \ln n - n} \int_{-\infty}^{\infty} e^{-y^2/(2n)}\, dy = e^{n\ln n - n}\sqrt{2\pi n} = \sqrt{2\pi n}\, n^n e^{-n},$$

which is Stirling's approximation (18.160). ◄

18.12.2 The beta function

The *beta function* is defined by

$$B(m,n) = \int_0^1 x^{m-1}(1-x)^{n-1}\, dx, \tag{18.162}$$

which converges for $m > 0$, $n > 0$, where m and n are, in general, real numbers. By letting $x = 1 - y$ in (18.162) it is easy to show that $B(m,n) = B(n,m)$. Other useful representations of the beta function may be obtained by suitable changes of variable. For example, putting $x = (1+y)^{-1}$ in (18.162), we find that

$$B(m,n) = \int_0^{\infty} \frac{y^{n-1}\, dy}{(1+y)^{m+n}}. \tag{18.163}$$

Alternatively, if we let $x = \sin^2\theta$ in (18.162), we obtain immediately

$$B(m,n) = 2\int_0^{\pi/2} \sin^{2m-1}\theta\, \cos^{2n-1}\theta\, d\theta. \tag{18.164}$$

The beta function may also be written in terms of the gamma function as

$$B(m,n) = \frac{\Gamma(m)\Gamma(n)}{\Gamma(m+n)}. \tag{18.165}$$

►*Prove the result (18.165).*

Using (18.157), we have

$$\begin{aligned}\Gamma(n)\Gamma(m) &= 4\int_0^{\infty} x^{2n-1}e^{-x^2}\, dx \int_0^{\infty} y^{2m-1}e^{-y^2}\, dy\\ &= 4\int_0^{\infty}\int_0^{\infty} x^{2n-1}y^{2m-1}e^{-(x^2+y^2)}\, dx\, dy.\end{aligned}$$

Changing variables to plane polar coordinates (ρ, ϕ) given by $x = \rho\cos\phi$, $y = \rho\sin\phi$, we obtain

$$\begin{aligned}\Gamma(n)\Gamma(m) &= 4\int_0^{\pi/2}\int_0^{\infty} \rho^{2(m+n-1)}e^{-\rho^2}\sin^{2m-1}\phi\,\cos^{2n-1}\phi\,\rho\,d\rho\,d\phi \\ &= 4\int_0^{\pi/2}\sin^{2m-1}\phi\,\cos^{2n-1}\phi\,d\phi\int_0^{\infty}\rho^{2(m+n)-1}e^{-\rho^2}\,d\rho \\ &= B(m,n)\Gamma(m+n),\end{aligned}$$

where in the last line we have used the results (18.157) and (18.164). ◄

The result (18.165) is useful in proving the identity (18.158) satisfied by the gamma function, since

$$\Gamma(n)\Gamma(1-n) = B(1-n,n) = \int_0^{\infty}\frac{y^{n-1}\,dy}{1+y},$$

where, in the second equality, we have used the integral representation (18.163). For $0 < n < 1$ this integral can be evaluated using contour integration and has the value $\pi/(\sin n\pi)$ (see exercise 24.19), thereby proving result (18.158) for this range of n. Extensions to other ranges require more sophisticated methods.

18.12.3 The incomplete gamma function

In the definition (18.153) of the gamma function, we may divide the range of integration into two parts and write

$$\Gamma(n) = \int_0^{x} u^{n-1}e^{-u}\,du + \int_x^{\infty} u^{n-1}e^{-u}\,du \equiv \gamma(n,x) + \Gamma(n,x), \tag{18.166}$$

whereby we have defined the *incomplete gamma functions* $\gamma(n,x)$ and $\Gamma(n,x)$, respectively. The choice of which of these two functions to use is merely a matter of convenience.

►*Show that if n is a positive integer*

$$\Gamma(n,x) = (n-1)!e^{-x}\sum_{k=0}^{n-1}\frac{x^k}{k!}.$$

From (18.166), on integrating by parts we find

$$\begin{aligned}\Gamma(n,x) = \int_x^{\infty} u^{n-1}e^{-u}du &= x^{n-1}e^{-x} + (n-1)\int_x^{\infty} u^{n-2}e^{-u}du \\ &= x^{n-1}e^{-x} + (n-1)\Gamma(n-1,x),\end{aligned}$$

which is valid for arbitrary n. If n is an integer, however, we obtain

$$\begin{aligned}\Gamma(n,x) &= e^{-x}[x^{n-1} + (n-1)x^{n-2} + (n-1)(n-2)x^{n-3} + \cdots + (n-1)!] \\ &= (n-1)!\,e^{-x}\sum_{k=0}^{n-1}\frac{x^k}{k!},\end{aligned}$$

which is the required result. ◀

We note that is it conventional to define, in addition, the functions

$$P(a,x) \equiv \frac{\gamma(a,x)}{\Gamma(a)}, \qquad Q(a,x) \equiv \frac{\Gamma(a,x)}{\Gamma(a)},$$

which are also often called incomplete gamma functions; it is clear that $Q(a,x) = 1 - P(a,x)$.

18.12.4 The error function

Finally, we mention the *error function*, which is encountered in probability theory and in the solutions of some partial differential equations. The error function is related to the incomplete gamma function by $\text{erf}(x) = \gamma(\frac{1}{2}, x^2)/\sqrt{\pi}$ and is thus given by

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2}\,du = 1 - \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2}\,du. \tag{18.167}$$

From this definition we can easily see that

$$\text{erf}(0) = 0, \qquad \text{erf}(\infty) = 1, \qquad \text{erf}(-x) = -\text{erf}(x).$$

By making the substitution $y = \sqrt{2}u$ in (18.167), we find

$$\text{erf}(x) = \sqrt{\frac{2}{\pi}} \int_0^{\sqrt{2}x} e^{-y^2/2}\,dy.$$

The cumulative probability function $\Phi(x)$ for the standard Gaussian distribution (discussed in section 30.9.1) may be written in terms of the error function as follows:

$$\begin{aligned}\Phi(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-y^2/2}\,dy \\ &= \frac{1}{2} + \frac{1}{\sqrt{2\pi}} \int_0^x e^{-y^2/2}\,dy \\ &= \frac{1}{2} + \frac{1}{2}\text{erf}\left(\frac{x}{\sqrt{2}}\right).\end{aligned}$$

It is also sometimes useful to define the *complementary error function*

$$\text{erfc}(x) = 1 - \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2}\,du = \frac{\Gamma(\frac{1}{2}, x^2)}{\sqrt{\pi}}. \tag{18.168}$$

18.13 Exercises

18.1 Use the explicit expressions

$$Y_0^0 = \sqrt{\tfrac{1}{4\pi}}, \qquad Y_1^0 = \sqrt{\tfrac{3}{4\pi}}\cos\theta,$$

$$Y_1^{\pm 1} = \mp\sqrt{\tfrac{3}{8\pi}}\sin\theta\exp(\pm i\phi), \qquad Y_2^0 = \sqrt{\tfrac{5}{16\pi}}(3\cos^2\theta - 1),$$

$$Y_2^{\pm 1} = \mp\sqrt{\tfrac{15}{8\pi}}\sin\theta\cos\theta\exp(\pm i\phi), \qquad Y_2^{\pm 2} = \sqrt{\tfrac{15}{32\pi}}\sin^2\theta\exp(\pm 2i\phi),$$

to verify for $\ell = 0, 1, 2$ that

$$\sum_{m=-\ell}^{\ell} |Y_\ell^m(\theta,\phi)|^2 = \frac{2\ell+1}{4\pi},$$

and so is independent of the values of θ and ϕ. This is true for any ℓ, but a general proof is more involved. This result helps to reconcile intuition with the apparently arbitrary choice of polar axis in a general quantum mechanical system.

18.2 Express the function

$$f(\theta,\phi) = \sin\theta[\sin^2(\theta/2)\cos\phi + i\cos^2(\theta/2)\sin\phi] + \sin^2(\theta/2)$$

as a sum of spherical harmonics.

18.3 Use the generating function for the Legendre polynomials $P_n(x)$ to show that

$$\int_0^1 P_{2n+1}(x)\,dx = (-1)^n \frac{(2n)!}{2^{2n+1}n!(n+1)!}$$

and that, except for the case $n = 0$,

$$\int_0^1 P_{2n}(x)\,dx = 0.$$

18.4 Carry through the following procedure as a proof of the result

$$I_n = \int_{-1}^{1} P_n(z)P_n(z)\,dz = \frac{2}{2n+1}.$$

(a) Square both sides of the generating-function definition of the Legendre polynomials,

$$(1 - 2zh + h^2)^{-1/2} = \sum_{n=0}^{\infty} P_n(z)h^n.$$

(b) Express the RHS as a sum of powers of h, obtaining expressions for the coefficients.
(c) Integrate the RHS from -1 to 1 and use the orthogonality property of the Legendre polynomials.
(d) Similarly integrate the LHS and expand the result in powers of h.
(e) Compare coefficients.

18.5 The Hermite polynomials $H_n(x)$ may be defined by

$$\Phi(x,h) = \exp(2xh - h^2) = \sum_{n=0}^{\infty} \frac{1}{n!}H_n(x)h^n.$$

Show that

$$\frac{\partial^2\Phi}{\partial x^2} - 2x\frac{\partial\Phi}{\partial x} + 2h\frac{\partial\Phi}{\partial h} = 0,$$

and hence that the $H_n(x)$ satisfy the Hermite equation

$$y'' - 2xy' + 2ny = 0,$$

where n is an integer ≥ 0.

Use Φ to prove that

(a) $H_n'(x) = 2nH_{n-1}(x)$,
(b) $H_{n+1}(x) - 2xH_n(x) + 2nH_{n-1}(x) = 0$.

18.6 A charge $+2q$ is situated at the origin and charges of $-q$ are situated at distances $\pm a$ from it along the polar axis. By relating it to the generating function for the Legendre polynomials, show that the electrostatic potential Φ at a point (r, θ, ϕ) with $r > a$ is given by

$$\Phi(r, \theta, \phi) = \frac{2q}{4\pi\epsilon_0 r} \sum_{s=1}^{\infty} \left(\frac{a}{r}\right)^{2s} P_{2s}(\cos\theta).$$

18.7 For the associated Laguerre polynomials, carry through the following exercises.

(a) Prove the Rodrigues' formula

$$L_n^m(x) = \frac{e^x x^{-m}}{n!} \frac{d^n}{dx^n}(x^{n+m}e^{-x}),$$

taking the polynomials to be defined by

$$L_n^m(x) = \sum_{k=0}^{n} (-1)^k \frac{(n+m)!}{k!(n-k)!(k+m)!} x^k.$$

(b) Prove the recurrence relations

$$(n+1)L_{n+1}^m(x) = (2n+m+1-x)L_n^m(x) - (n+m)L_{n-1}^m(x),$$

$$x(L_n^m)'(x) = nL_n^m(x) - (n+m)L_{n-1}^m(x),$$

but this time taking the polynomial as defined by

$$L_n^m(x) = (-1)^m \frac{d^m}{dx^m} L_{n+m}(x)$$

or the generating function.

18.8 The quantum mechanical wavefunction for a one-dimensional simple harmonic oscillator in its nth energy level is of the form

$$\psi(x) = \exp(-x^2/2)H_n(x),$$

where $H_n(x)$ is the nth Hermite polynomial. The generating function for the polynomials is

$$G(x, h) = e^{2hx-h^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} h^n.$$

(a) Find $H_i(x)$ for $i = 1, 2, 3, 4$.
(b) Evaluate by direct calculation

$$\int_{-\infty}^{\infty} e^{-x^2} H_p(x) H_q(x)\, dx,$$

(i) for $p = 2$, $q = 3$; (ii) for $p = 2$, $q = 4$; (iii) for $p = q = 3$. Check your answers against the expected values $2^p\, p! \sqrt{\pi}\, \delta_{pq}$.

[You will find it convenient to use

$$\int_{-\infty}^{\infty} x^{2n} e^{-x^2}\, dx = \frac{(2n)!\sqrt{\pi}}{2^{2n} n!}$$

for integer $n \geq 0$.]

18.9 By initially writing $y(x)$ as $x^{1/2} f(x)$ and then making subsequent changes of variable, reduce Stokes' equation,

$$\frac{d^2 y}{dx^2} + \lambda x y = 0,$$

to Bessel's equation. Hence show that a solution that is finite at $x = 0$ is a multiple of $x^{1/2} J_{1/3}(\frac{2}{3}\sqrt{\lambda x^3})$.

18.10 By choosing a suitable form for h in their generating function,

$$G(z, h) = \exp\left[\frac{z}{2}\left(h - \frac{1}{h}\right)\right] = \sum_{n=-\infty}^{\infty} J_n(z) h^n,$$

show that integral repesentations of the Bessel functions of the first kind are given, for integral m, by

$$J_{2m}(z) = \frac{(-1)^m}{\pi} \int_0^{2\pi} \cos(z\cos\theta)\, \cos 2m\theta\, d\theta \qquad m \geq 1,$$

$$J_{2m+1}(z) = \frac{(-1)^{m+1}}{\pi} \int_0^{2\pi} \cos(z\cos\theta)\, \sin(2m+1)\theta\, d\theta \qquad m \geq 0.$$

18.11 Identify the series for the following hypergeometric functions, writing them in terms of better known functions:

(a) $F(a, b, b; z)$,
(b) $F(1, 1, 2; -x)$,
(c) $F(\frac{1}{2}, 1, \frac{3}{2}; -x^2)$,
(d) $F(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}; x^2)$,
(e) $F(-a, a, \frac{1}{2}; \sin^2 x)$; this is a much more difficult exercise.

18.12 By making the substitution $z = (1 - x)/2$ and suitable choices for a, b and c, convert the hypergeometric equation,

$$z(1-z)\frac{d^2 u}{dz^2} + [\,c - (a + b + 1)z\,]\frac{du}{dz} - abu = 0,$$

into the Legendre equation,

$$(1 - x^2)\frac{d^2 y}{dx^2} - 2x\frac{dy}{dx} + \ell(\ell + 1)y = 0.$$

Hence, using the hypergeometric series, generate the Legendre polynomials $P_\ell(x)$ for the integer values $\ell = 0, 1, 2, 3$. Comment on their normalisations.

18.13 Find a change of variable that will allow the integral

$$I = \int_1^{\infty} \frac{\sqrt{u - 1}}{(u + 1)^2}\, du$$

to be expressed in terms of the beta function, and so evaluate it.

18.14 Prove that, if m and n are both greater than -1, then

$$I = \int_0^{\infty} \frac{u^m}{(au^2 + b)^{(m+n+2)/2}}\, du = \frac{\Gamma[\,\frac{1}{2}(m+1)\,]\,\Gamma[\,\frac{1}{2}(n+1)\,]}{2a^{(m+1)/2}\, b^{(n+1)/2}\, \Gamma[\,\frac{1}{2}(m+n+2)\,]}.$$

Deduce the value of

$$J = \int_0^\infty \frac{(u+2)^2}{(u^2+4)^{5/2}}\, du.$$

18.15 The complex function $z!$ is defined by

$$z! = \int_0^\infty u^z e^{-u}\, du \qquad \text{for } \operatorname{Re} z > -1.$$

For $\operatorname{Re} z \le -1$ it is defined by

$$z! = \frac{(z+n)!}{(z+n)(z+n-1)\cdots(z+1)},$$

where n is any (positive) integer $> -\operatorname{Re} z$. Being the ratio of two polynomials, $z!$ is analytic everywhere in the finite complex plane except at the poles that occur when z is a negative integer.

(a) Show that the definition of $z!$ for $\operatorname{Re} z \le -1$ is independent of the value of n chosen.
(b) Prove that the residue of $z!$ at the pole $z = -m$, where m is an integer > 0, is $(-1)^{m-1}/(m-1)!$.

18.16 For $-1 < \operatorname{Re} z < 1$, use the definition and value of the beta function to show that

$$z!(-z)! = \int_0^\infty \frac{u^z}{(1+u)^2}\, du.$$

Contour integration gives the value of the integral on the RHS of the above equation as $\pi z \operatorname{cosec} \pi z$. Use this to deduce the value of $(-\frac{1}{2})!$.

18.17 The integral

$$I = \int_{-\infty}^\infty \frac{e^{-k^2}}{k^2+a^2}\, dk, \qquad (*)$$

in which $a > 0$, occurs in some statistical mechanics problems. By first considering the integral

$$J = \int_0^\infty e^{iu(k+ia)}\, du,$$

and a suitable variation of it, show that $I = (\pi/a)\exp(a^2)\operatorname{erfc}(a)$, where $\operatorname{erfc}(x)$ is the complementary error function.

18.18 Consider two series expansions of the error function as follows.

(a) Obtain a series expansion of the error function $\operatorname{erf}(x)$ in ascending powers of x. How many terms are needed to give a value correct to four significant figures for $\operatorname{erf}(1)$?
(b) Obtain an asymptotic expansion that can be used to estimate $\operatorname{erfc}(x)$ for large x (> 0) in the form of a series

$$\operatorname{erfc}(x) = R(x) = e^{-x^2} \sum_{n=0}^\infty \frac{a_n}{x^n}.$$

Consider what bounds can be put on the estimate and at what point the infinite series should be terminated in a practical estimate. In particular, estimate $\operatorname{erfc}(1)$ and test the answer for compatibility with that in part (a).

18.19 For the functions $M(a, c; z)$ that are the solutions of the confluent hypergeometric equation,

(a) use their series representation to prove that

$$b\frac{d}{dz}M(a,c;z) = a\,M(a+1,c+1;z);$$

(b) use an integral representation to prove that

$$M(a,c;z) = e^z M(c-a,c;-z).$$

18.20 The Bessel function $J_\nu(z)$ can be considered as a special case of the solution $M(a,c;z)$ of the confluent hypergeometric equation, the connection being

$$\lim_{a\to\infty}\frac{M(a,\nu+1;-z/a)}{\Gamma(\nu+1)} = z^{-\nu/2}J_\nu(2\sqrt{z}).$$

Prove this equality by writing each side in terms of an infinite series and showing that the series are the same.

18.21 Find the differential equation satisfied by the function $y(x)$ defined by

$$y(x) = Ax^{-n}\int_0^x e^{-t}t^{n-1}\,dt \equiv Ax^{-n}\gamma(n,x),$$

and, by comparing it with the confluent hypergeometric function, express y as a multiple of the solution $M(a,c;z)$ of that equation. Determine the value of A that makes y equal to M.

18.22 Show, from its definition, that the Bessel function of the second kind, and of integral order ν, can be written as

$$Y_\nu(z) = \frac{1}{\pi}\left[\frac{\partial J_\mu(z)}{\partial\mu} - (-1)^\nu\frac{\partial J_{-\mu}(z)}{\partial\mu}\right]_{\mu=\nu}.$$

Using the explicit series expression for $J_\mu(z)$, show that $\partial J_\mu(z)/\partial\mu$ can be written as

$$J_\nu(z)\ln\left(\frac{z}{2}\right) + g(\nu,z),$$

and deduce that $Y_\nu(z)$ can be expressed as

$$Y_\nu(z) = \frac{2}{\pi}J_\nu(z)\ln\left(\frac{z}{2}\right) + h(\nu,z),$$

where $h(\nu,z)$, like $g(\nu,z)$, is a power series in z.

18.23 Prove two of the properties of the incomplete gamma function $P(a,x^2)$ as follows.

(a) By considering its form for a suitable value of a, show that the error function can be expressed as a particular case of the incomplete gamma function.

(b) The Fresnel integrals, of importance in the study of the diffraction of light, are given by

$$C(x) = \int_0^x \cos\left(\frac{\pi}{2}t^2\right)dt, \qquad S(x) = \int_0^x \sin\left(\frac{\pi}{2}t^2\right)dt.$$

Show that they can be expressed in terms of the error function by

$$C(x) + iS(x) = A\,\mathrm{erf}\left[\frac{\sqrt{\pi}}{2}(1-i)x\right],$$

where A is a (complex) constant, which you should determine. Hence express $C(x)+iS(x)$ in terms of the incomplete gamma function.

18.24 The solutions $y(x, a)$ of the equation

$$\frac{d^2y}{dx^2} - (\tfrac{1}{4}x^2 + a)y = 0 \qquad (*)$$

are known as parabolic cylinder functions.

(a) If $y(x, a)$ is a solution of $(*)$, determine which of the following are also solutions: (i) $y(a, -x)$, (ii) $y(-a, x)$, (iii) $y(a, ix)$ and (iv) $y(-a, ix)$.

(b) Show that one solution of $(*)$, even in x, is

$$y_1(x, a) = e^{-x^2/4} M(\tfrac{1}{2}a + \tfrac{1}{4}, \tfrac{1}{2}, \tfrac{1}{2}x^2),$$

where $M(\alpha, c, z)$ is the confluent hypergeometric function satisfying

$$z\frac{d^2M}{dz^2} + (c - z)\frac{dM}{dz} - \alpha M = 0.$$

You may assume (or prove) that a second solution, odd in x, is given by $y_2(x, a) = xe^{-x^2/4} M(\tfrac{1}{2}a + \tfrac{3}{4}, \tfrac{3}{2}, \tfrac{1}{2}x^2)$.

(c) Find, as an infinite series, an explicit expression for $e^{x^2/4} y_1(x, a)$.

(d) Using the results from part (a), show that $y_1(x, a)$ can also be written as

$$y_1(x, a) = e^{x^2/4} M(-\tfrac{1}{2}a + \tfrac{1}{4}, \tfrac{1}{2}, -\tfrac{1}{2}x^2).$$

(e) By making a suitable choice for a deduce that

$$1 + \sum_{n=1}^{\infty} \frac{b_n\, x^{2n}}{(2n)!} = e^{x^2/2}\left(1 + \sum_{n=1}^{\infty} \frac{(-1)^n\, b_n\, x^{2n}}{(2n)!}\right),$$

where $b_n = \prod_{r=1}^{n}(2r - \tfrac{3}{2})$.

18.14 Hints and answers

18.1 Note that taking the square of the modulus eliminates all mention of ϕ.

18.3 Integrate both sides of the generating function definition from $x = 0$ to $x = 1$, and then expand the resulting term, $(1 + h^2)^{1/2}$, using a binomial expansion. Show that ${}^{1/2}C_m$ can be written as $[(-1)^{m-1}(2m-2)!]/[2^{2m-1}m!(m-1)!]$.

18.5 Prove the stated equation using the explicit closed form of the generating function. Then substitute the series and require the coefficient of each power of h to vanish. (b) Differentiate result (a) and then use (a) again to replace the derivatives.

18.7 (a) Write the result of using Leibnitz' theorem on the product of x^{n+m} and e^{-x} as a finite sum, evaluate the separated derivatives, and then re-index the summation. (b) For the first recurrence relation, differentiate the generating function with respect to h and then use the generating function again to replace the exponential. Equating coefficients of h^n then yields the result. For the second, differentiate the corresponding relationship for the ordinary Laguerre polynomials m times.

18.9 $x^2 f'' + xf' + (\lambda x^3 - \tfrac{1}{4})f = 0$. Then, in turn, set $x^{3/2} = u$, and $\tfrac{2}{3}\lambda^{1/2}u = v$; then v satisfies Bessel's equation with $\nu = \tfrac{1}{3}$.

18.11 (a) $(1 - z)^{-a}$. (b) $x^{-1}\ln(1 + x)$. (c) Compare the calculated coefficients with those of $\tan^{-1} x$. $F(\tfrac{1}{2}, 1, \tfrac{3}{2}; -x^2) = x^{-1}\tan^{-1} x$. (d) $x^{-1}\sin^{-1} x$. (e) Note that a term containing x^{2n} can only arise from the first $n+1$ terms of an expansion in powers of $\sin^2 x$; make a few trials. $F(-a, a, \tfrac{1}{2}; \sin^2 x) = \cos 2ax$.

18.13 Looking for $f(x) = u$ such that $u + 1$ is an inverse power of x with $f(0) = \infty$ and $f(1) = 1$ leads to $f(x) = 2x^{-1} - 1$. $I = B(\tfrac{1}{2}, \tfrac{3}{2})/\sqrt{2} = \pi/(2\sqrt{2})$.

18.15 (a) Show that the ratio of two definitions based on m and n, with $m > n > -\text{Re}\, z$, is unity, independent of the actual values of m and n.
(b) Consider the limit as $z \to -m$ of $(z+m)z!$, with the definition of $z!$ based on n where $n > m$.

18.17 Express the integrand in partial fractions and use J, as given, and $J' = \int_0^\infty \exp[-iu(k-ia)]\, du$ to express I as the sum of two double integral expressions. Reduce them using the standard Gaussian integral, and then make a change of variable $2v = u + 2a$.

18.19 (b) Using the representation

$$M(a, b; z) = \frac{\Gamma(b)}{\Gamma(b-a)\,\Gamma(a)} \int_0^1 e^{zt}\, t^{a-1}\, (1-t)^{b-a-1}\, dt$$

allows the equality to be established, without actual integration, by changing the integration variable to $s = 1 - t$.

18.21 Calculate $y'(x)$ and $y''(x)$ and then eliminate $x^{-1}e^{-x}$ to obtain $xy'' + (n+1+x)y' + ny = 0$; $M(n, n+1; -x)$. Comparing the expansion of the hypergeometric series with the result of term by term integration of the expansion of the integrand shows that $A = n$.

18.23 (a) If the dummy variable in the incomplete gamma function is t, make the change of variable $y = +\sqrt{t}$. Now choose a so that $2(a-1)+1 = 0$; $\text{erf}(x) = P(\frac{1}{2}, x^2)$.
(b) Change the integration variable u in the standard representation of the RHS to s, given by $u = \frac{1}{2}\sqrt{\pi}(1-i)s$, and note that $(1-i)^2 = -2i$. $A = (1+i)/2$. From part (a), $C(x) + iS(x) = \frac{1}{2}(1+i)P(\frac{1}{2}, -\frac{1}{2}\pi i\, x^2)$.

19

Quantum operators

Although the previous chapter was principally concerned with the use of linear operators and their eigenfunctions in connection with the solution of given differential equations, it is of interest to study the properties of the operators themselves and determine which of them follow purely from the nature of the operators, without reference to specific forms of eigenfunctions.

19.1 Operator formalism

The results we will obtain in this chapter have most of their applications in the field of quantum mechanics and our descriptions of the methods will reflect this. In particular, when we discuss a function ψ that depends upon variables such as space coordinates and time, and possibly also on some non-classical variables, ψ will usually be a quantum-mechanical wavefunction that is being used to describe the state of a physical system. For example, the value of $|\psi|^2$ for a particular set of values of the variables is interpreted in quantum mechanics as being the probability that the system's variables have that set of values.

To this end, we will be no more specific about the functions involved than attaching just enough labels to them that a particular function, or a particular set of functions, is identified. A convenient notation for this kind of approach is that already hinted at, but not specifically stated, in subsection 17.1, where the definition of an inner product is given. This notation, often called the Dirac notation, denotes a state whose wavefunction is ψ by $|\,\psi\rangle$; since ψ belongs to a vector space of functions, $|\,\psi\rangle$ is known as a *ket vector*. Ket vectors, or simply kets, must not be thought of as completely analogous to physical vectors. Quantum mechanics associates the same physical state with $ke^{i\theta}|\,\psi\rangle$ as it does with $|\,\psi\rangle$ for all real k and θ and so there is no loss of generality in taking k as 1 and θ as 0. On the other hand, the combination $c_1|\,\psi_1\rangle + c_2|\,\psi_2\rangle$, where $|\,\psi_1\rangle$ and $|\,\psi_2\rangle$

represent different states, is a ket that represents a continuum of different states as the complex numbers c_1 and c_2 are varied.

If we need to specify a state more closely – say we know that it corresponds to a plane wave with a wave number whose magnitude is k – then we indicate this with a label; the corresponding ket vector would be written as $|\,k\rangle$. If we also knew the direction of the wave then $|\,\mathbf{k}\rangle$ would be the appropriate form. Clearly, in general, the more labels we include, the more precisely the corresponding state is specified.

The Dirac notation for the Hermitian conjugate (dual vector) of the ket vector $|\,\psi\rangle$ is written as $\langle\psi|$ and is known as a *bra vector*; the wavefunction describing this state is ψ^*, the complex conjugate of ψ. The inner product of two wavefunctions $\int \psi^*\phi\, dv$ is then denoted by $\langle\psi|\,\phi\rangle$ or, more generally if a non-unit weight function ρ is involved, by

$$\langle\psi|\,\rho|\,\phi\rangle, \quad \text{evaluated as} \quad \int \psi^*(\mathbf{r})\phi(\mathbf{r})\rho(\mathbf{r})\,d\mathbf{r}. \tag{19.1}$$

Given the (contrived) names for the two sorts of vectors, an inner product like $\langle\psi|\,\phi\rangle$ becomes a particular type of 'bra(c)ket'. Despite its somewhat whimsical construction, this type of quantity has a fundamental role to play in the interpretation of quantum theory, because expectation values, probabilities and transition rates are all expressed in terms of them. For physical states the inner product of the corresponding ket with itself, with or without an explicit weight function, is non-zero, and it is usual to take

$$\langle\psi|\psi\rangle = 1.$$

Although multiplying a ket vector by a constant does not change the state described by the vector, acting upon it with a more general linear operator A results (in general) in a ket describing a different state. For example, if ψ is a state that is described in one-dimensional x-space by the wavefunction $\psi(x) = \exp(-x^2)$ and A is the differential operator $\partial/\partial x$, then

$$|\,\psi_1\rangle = A|\,\psi\rangle \equiv |\,A\psi\rangle$$

is the ket associated with the state whose wavefunction is $\psi_1(x) = -2x\exp(-x^2)$, clearly a different state. This allows us to attach a meaning to an expression such as $\langle\phi|A|\,\psi\rangle$ through the equation

$$\langle\phi|A|\,\psi\rangle = \langle\phi|\,\psi_1\rangle, \tag{19.2}$$

i.e. it is the inner product of $|\,\psi_1\rangle$ and $|\,\phi\rangle$. We have already used this notation in equation (19.1), but there the effect of the operator A was merely multiplication by a weight function.

If it should happen that the effect of an operator acting upon a particular ket is to produce a scalar multiple of that ket, i.e.

$$A|\,\psi\rangle = \lambda|\,\psi\rangle, \tag{19.3}$$

then, just as for matrices and differential equations, $|\,\psi\rangle$ is called an *eigenket* or, more usually, an *eigenstate* of A, with corresponding eigenvalue λ; to mark this special property the state will normally be denoted by $|\,\lambda\rangle$, rather than by the more general $|\,\psi\rangle$. Taking the Hermitian conjugate of this ket vector eigenequation gives a bra vector equation,

$$\langle\psi|A^\dagger = \lambda^*\langle\psi|. \tag{19.4}$$

It should be noted that the complex conjugate of the eigenvalue appears in this equation. Should the action of A on $|\psi\rangle$ produce an unphysical state (usually one whose wavefunction is identically zero, and is therefore unacceptable as a quantum-mechanical wavefunction because of the required probability interpretation) we denote the result either by 0 or by the ket vector $|\,\emptyset\,\rangle$ according to context. Formally, $|\,\emptyset\,\rangle$ can be considered as an eigenket of any operator, but one for which the eigenvalue is always zero.

If an operator A is Hermitian ($A^\dagger = A$) then its eigenvalues are real and the eigenstates can be chosen to be orthogonal; this can be shown in the same way as in chapter 17 (but using a different notation). As indicated there, the reality of their eigenvalues is one reason why Hermitian operators form the basis of measurement in quantum mechanics; in that formulation of physics, the eigenvalues of an operator are the *only* possible values that can be obtained when a measurement of the physical quantity corresponding to the operator is made. Actual individual measurements must always result in real values, even if they are combined in a complex form ($x + iy$ or $re^{i\theta}$) for final presentation or analysis, and using only Hermitian operators ensures this. The proof of the reality of the eigenvalues using the Dirac notation is given below in a worked example.

In the same notation the Hermitian property of an operator A is represented by the double equality

$$\langle A\,\phi|\psi\rangle = \langle\phi|A|\,\psi\rangle = \langle\phi|A\,\psi\rangle.$$

It should be remembered that the definition of an Hermitian operator involves specifying boundary conditions that the wavefunctions considered must satisfy. Typically, they are that the wavefunctions vanish for large values of the spatial variables upon which they depend; this deals with most physical systems since they are nearly all formally infinite in extent. Some model systems require the wavefunction to be periodic or to vanish at finite values of a spatial variable.

Depending on the nature of the physical system, the eigenvalues of a particular linear operator may be discrete, part of a continuum, or a mixture of both. For example, the energy levels of the bound proton–electron system (the hydrogen atom) are discrete, but if the atom is ionised and the electron is free, the energy spectrum of the system is continuous. This system has discrete negative and continuous positive eigenvalues for the operator corresponding to the total energy (the Hamiltonian).

► *Using the Dirac notation, show that the eigenvalues of an Hermitian operator are real.*

Let $|\,a\rangle$ be an eigenstate of Hermitian operator A corresponding to eigenvalue a, then

$$\begin{aligned} A|\,a\rangle &= a|\,a\rangle, \\ \Rightarrow \quad \langle a|A|\,a\rangle &= \langle a|a|\,a\rangle = a\langle a|\,a\rangle, \\ &\text{and} \\ \langle a|A^\dagger &= a^*\langle a|, \\ \Rightarrow \quad \langle a|A^\dagger|\,a\rangle &= a^*\langle a|\,a\rangle, \\ \langle a|A|\,a\rangle &= a^*\langle a|\,a\rangle, \quad \text{since } A \text{ is Hermitian.} \end{aligned}$$

Hence,

$$\begin{aligned} (a-a^*)\langle a|\,a\rangle &= 0, \\ \Rightarrow \quad a &= a^*, \text{ since } \langle a|\,a\rangle \neq 0. \end{aligned}$$

Thus a is real. ◄

It is not our intention to describe the complete axiomatic basis of quantum mechanics, but rather to show what can be learned about linear operators, and in particular about their eigenvalues, without recourse to explicit wavefunctions on which the operators act.

Before we proceed to do that, we close this subsection with a number of results, expressed in Dirac notation, that the reader should verify by inspection or by following the lines of argument sketched in the statements. Where a sum over a complete set of eigenvalues is shown, it should be replaced by an integral for those parts of the eigenvalue spectrum that are continuous. With the notation that $|a_n\rangle$ is an eigenstate of Hermitian operator A with non-degenerate eigenvalue a_n (or, if a_n is k-fold degenerate, then a set of k mutually orthogonal eigenstates has been constructed and the states relabelled), we have the following results.

$$A|\,a_n\rangle = a_n|\,a_n\rangle,$$

$$\langle a_m|a_n\rangle = \delta_{mn} \quad \text{(orthonormality of eigenstates)}, \tag{19.5}$$

$$A(c_n|\,a_n\rangle + c_m|\,a_m\rangle) = c_n a_n|\,a_n\rangle + c_m a_m|\,a_m\rangle \quad \text{(linearity)}. \tag{19.6}$$

The definitions of the sum and product of two operators are

$$(A+B)|\,\psi\rangle \equiv A|\,\psi\rangle + B|\,\psi\rangle, \tag{19.7}$$

$$AB|\,\psi\rangle \equiv A(B|\,\psi\rangle) \quad (\neq BA|\,\psi\rangle \text{ in general}), \tag{19.8}$$

$$\Rightarrow \quad A^p|\,a_n\rangle = a_n^p|\,a_n\rangle. \tag{19.9}$$

If $A|\,a_n\rangle = a|\,a_n\rangle$ for all $N_1 \le n \le N_2$, then

$$|\,\psi\rangle = \sum_{n=N_1}^{N_2} d_n|\,a_n\rangle \text{ satisfies } A|\,\psi\rangle = a|\,\psi\rangle \text{ for any set of } d_i.$$

For a general state $|\,\psi\rangle$,

$$|\,\psi\rangle = \sum_{n=0}^{\infty} c_n|\,a_n\rangle, \text{ where } c_n = \langle a_n|\psi\rangle. \tag{19.10}$$

This can also be expressed as the operator identity,

$$1 = \sum_{n=0}^{\infty} |\,a_n\rangle\,\langle a_n|, \tag{19.11}$$

in the sense that

$$|\,\psi\rangle = 1\,|\,\psi\rangle = \sum_{n=0}^{\infty} |\,a_n\rangle\,\langle a_n|\psi\rangle = \sum_{n=0}^{\infty} c_n|\,a_n\rangle.$$

It also follows that

$$1 = \langle\psi|\psi\rangle = \left(\sum_{m=0}^{\infty} c_m^*\langle a_m|\right)\left(\sum_{n=0}^{\infty} c_n|a_n\rangle\right) = \sum_{m,n}^{\infty} c_m^* c_n \delta_{mn} = \sum_{n=0}^{\infty} |c_n|^2. \tag{19.12}$$

Similarly, the expectation value of the physical variable corresponding to A is

$$\begin{aligned}\langle\psi|A|\,\psi\rangle &= \sum_{m,n}^{\infty} c_m^*\langle a_m|\,A|\,a_n\rangle c_n = \sum_{m,n}^{\infty} c_m^*\langle a_m|\,a_n|\,a_n\rangle c_n \\ &= \sum_{m,n}^{\infty} c_m^* c_n a_n \delta_{mn} = \sum_{n=0}^{\infty} |c_n|^2 a_n.\end{aligned} \tag{19.13}$$

19.1.1 Commutation and commutators

As has been noted above, the product AB of two linear operators may or may not be equal to the product BA. That is

$$AB|\,\psi\rangle \text{ is not necessarily equal to } BA|\,\psi\rangle.$$

If A and B are both purely multiplicative operators, multiplication by $f(\mathbf{r})$ and $g(\mathbf{r})$ say, then clearly the order of the operations is immaterial, the result $|\,f(\mathbf{r})g(\mathbf{r})\psi\rangle$ being obtained in both cases. However, consider a case in which A is the differential operator $\partial/\partial x$ and B is the operator 'multiply by x'. Then the wavefunction describing $AB|\,\psi\rangle$ is

$$\frac{\partial}{\partial x}(x\psi(x)) = \psi(x) + x\frac{\partial\psi}{\partial x},$$

whilst that for $BA|\psi\rangle$ is simply

$$x\frac{\partial \psi}{\partial x},$$

which is not the same.

If the result

$$AB|\psi\rangle = BA|\psi\rangle$$

is true for *all* ket vectors $|\psi\rangle$, then A and B are said to *commute*; otherwise they are non-commuting operators.

A convenient way to express the commutation properties of two linear operators is to define their *commutator*, $[A, B]$, by

$$[A, B]\,|\psi\rangle \equiv AB|\psi\rangle - BA|\psi\rangle. \tag{19.14}$$

Clearly two operators that commute have a zero commutator. But, for the example given above we have that

$$\left[\frac{\partial}{\partial x}, x\right]\psi(x) = \left(\psi(x) + x\frac{\partial \psi}{\partial x}\right) - \left(x\frac{\partial \psi}{\partial x}\right) = \psi(x) = 1 \times \psi$$

or, more simply, that

$$\left[\frac{\partial}{\partial x}, x\right] = 1; \tag{19.15}$$

in words, the commutator of the differential operator $\partial/\partial x$ and the multiplicative operator x is the multiplicative operator 1. It should be noted that the order of the linear operators is important and that

$$[A, B] = -[B, A]. \tag{19.16}$$

Clearly any linear operator commutes with itself and some other obvious zero commutators (when operating on wavefunctions with 'reasonable' properties) are:

$[A, I]$, where I is the identity operator;
$[A^n, A^m]$, for any positive integers n and m;
$[A, p(A)]$, where $p(x)$ is any polynomial in x;
$[A, c]$, where A is any linear operator and c is any constant;
$[f(x), g(x)]$, where the functions are mutiplicative;
$[A(x), B(y)]$, where the operators act on different variables, with
$\left[\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right]$ as a specific example.

Simple identities amongst commutators include the following:

$$[A, B + C] = [A, B] + [A, C], \tag{19.17}$$

$$[A + B, C] = [A, C] + [B, C], \tag{19.18}$$

$$\begin{aligned} [A, BC] &= ABC - BCA + BAC - BAC \\ &= (AB - BA)C + B(AC - CA) \\ &= [A, B]C + B[A, C], \end{aligned} \tag{19.19}$$

$$[AB, C] = A[B, C] + [A, C]B. \tag{19.20}$$

►*If A and B are two linear operators that both commute with their commutator, prove that $[A, B^n] = nB^{n-1}[A, B]$ and that $[A^n, B] = nA^{n-1}[A, B]$.*

Define C_n by $C_n = [A, B^n]$. We aim to find a reduction formula for C_n:

$$\begin{aligned} C_n &= \left[A, B\,B^{n-1}\right] \\ &= [A, B]\,B^{n-1} + B\left[A, B^{n-1}\right], \text{ using (19.19),} \\ &= B^{n-1}[A, B] + B\left[A, B^{n-1}\right], \text{ since } [[A, B], B] = 0, \\ &= B^{n-1}[A, B] + BC_{n-1}, \text{ the required reduction formula,} \\ &= B^{n-1}[A, B] + B\{B^{n-2}[A, B] + BC_{n-2}\}, \text{ applying the formula,} \\ &= 2B^{n-1}[A, B] + B^2 C_{n-2} \\ &= \cdots \\ &= nB^{n-1}[A, B] + B^n C_0. \end{aligned}$$

However, $C_0 = [A, I] = 0$ and so $C_n = nB^{n-1}[A, B]$.

Using equation (19.16) and interchanging A and B in the result just obtained, we find

$$[A^n, B] = -[B, A^n] = -nA^{n-1}[B, A] = nA^{n-1}[A, B],$$

as stated in the question. ◄

As the power of a linear operator can be defined, so can its exponential; this situation parallels that for matrices, which are of course a particular set of operators that act upon state functions represented by vectors. The definition follows that for the exponential of a scalar or matrix, namely

$$\exp A = \sum_{n=0}^{\infty} \frac{A^n}{n!}. \tag{19.21}$$

Related functions of A, such as $\sin A$ and $\cos A$, can be defined in a similar way.

Since any linear operator commutes with itself, when two functions of it are combined in some way, the result takes a form similar to that for the corresponding functions of scalar quantities. Consider, for example, the function $f(A)$ defined by $f(A) = 2 \sin A \cos A$. Expressing $\sin A$ and $\cos A$ in terms of their defining series, we have

$$f(A) = 2\sum_{m=0}^{\infty} \frac{(-1)^m A^{2m+1}}{(2m+1)!} \sum_{n=0}^{\infty} \frac{(-1)^n A^{2n}}{(2n)!}.$$

Writing $m+n$ as r and replacing n by s, we have

$$\begin{aligned} f(A) &= 2\sum_{r=0}^{\infty} A^{2r+1} \left(\sum_{s=0}^{r} \frac{(-1)^{r-s}}{(2r-2s+1)!} \frac{(-1)^s}{(2s)!} \right) \\ &= 2\sum_{r=0}^{\infty} (-1)^r c_r A^{2r+1}, \end{aligned}$$

where

$$c_r = \sum_{s=0}^{r} \frac{1}{(2r-2s+1)!(2s)!} = \frac{1}{(2r+1)!} \sum_{s=0}^{r} {}^{2r+1}C_{2s}.$$

By adding the binomial expansions of $2^{2r+1} = (1+1)^{2r+1}$ and $0 = (1-1)^{2r+1}$, it can easily be shown that

$$2^{2r+1} = 2\sum_{s=0}^{r} {}^{2r+1}C_{2s} \quad \Rightarrow \quad c_r = \frac{2^{2r}}{(2r+1)!}.$$

It then follows that

$$2\sin A \cos A = 2\sum_{r=0}^{\infty} \frac{(-1)^r A^{2r+1} 2^{2r}}{(2r+1)!} = \sum_{r=0}^{\infty} \frac{(-1)^r (2A)^{2r+1}}{(2r+1)!} = \sin 2A,$$

a not unexpected result.

However, if two (or more) linear operators that do not commute are involved, combining functions of them is more complicated and the results less intuitively obvious. We take as a particular case the product of two exponential functions and, even then, take the simplified case in which each linear operator commutes with their commutator (so that we may use the results from the previous worked example).

►*If A and B are two linear operators that both commute with their commutator, show that*

$$\exp(A)\exp(B) = \exp(A + B + \tfrac{1}{2}[A, B]).$$

We first find the commutator of A and $\exp \lambda B$, where λ is a scalar quantity introduced for later algebraic convenience:

$$\begin{aligned}
\left[A, e^{\lambda B}\right] &= \left[A, \sum_{n=0}^{\infty} \frac{(\lambda B)^n}{n!}\right] = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!}\left[A, B^n\right] \\
&= \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} n B^{n-1}\left[A, B\right], \text{ using the earlier result,} \\
&= \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} n B^{n-1}\left[A, B\right] \\
&= \lambda \sum_{m=0}^{\infty} \frac{\lambda^m B^m}{m!}\left[A, B\right], \text{ writing } m = n-1, \\
&= \lambda e^{\lambda B}\left[A, B\right].
\end{aligned}$$

Now consider the derivative with respect to λ of the function

$$f(\lambda) = e^{\lambda A} e^{\lambda B} e^{-\lambda(A+B)}.$$

In the following calculation we use the fact that the derivative of $e^{\lambda C}$ is $Ce^{\lambda C}$; this is the same as $e^{\lambda C}C$, since any two functions of the same operator commute. Differentiating the three-factor product gives

$$\begin{aligned}
\frac{df}{d\lambda} &= e^{\lambda A} A e^{\lambda B} e^{-\lambda(A+B)} + e^{\lambda A} e^{\lambda B} B e^{-\lambda(A+B)} + e^{\lambda A} e^{\lambda B}(-A-B) e^{-\lambda(A+B)} \\
&= e^{\lambda A}(e^{\lambda B} A + \lambda e^{\lambda B}\left[A, B\right]) e^{-\lambda(A+B)} + e^{\lambda A} e^{\lambda B} B e^{-\lambda(A+B)} \\
&\qquad - e^{\lambda A} e^{\lambda B} A e^{-\lambda(A+B)} - e^{\lambda A} e^{\lambda B} B e^{-\lambda(A+B)} \\
&= e^{\lambda A} \lambda e^{\lambda B}\left[A, B\right] e^{-\lambda(A+B)} \\
&= \lambda\left[A, B\right] f(\lambda).
\end{aligned}$$

In the second line we have used the result obtained above to replace $Ae^{\lambda B}$, and in the last line have used the fact that $[A, B]$ commutes with each of A and B, and hence with any function of them.

Integrating this scalar differential equation with respect to λ and noting that $f(0) = 1$, we obtain

$$\ln f = \tfrac{1}{2}\lambda^2\left[A, B\right] \quad \Rightarrow \quad e^{\lambda A} e^{\lambda B} e^{-\lambda(A+B)} = f(\lambda) = e^{\frac{1}{2}\lambda^2[A,B]}.$$

Finally, post-multiplying both sides of the equation by $e^{\lambda(A+B)}$ and setting $\lambda = 1$ yields

$$e^A e^B = e^{\frac{1}{2}[A,B]+A+B}. \blacktriangleleft$$

19.2 Physical examples of operators

We now turn to considering some of the specific linear operators that play a part in the description of physical systems. In particular, we will examine the properties of some of those that appear in the quantum-mechanical description of the physical world.

As stated earlier, the operators corresponding to physical observables are restricted to Hermitian operators (which have real eigenvalues) as this ensures the reality of predicted values for experimentally measured quantities. The two basic quantum-mechanical operators are those corresponding to position **r** and momentum **p**. One prescription for making the transition from classical to quantum mechanics is to express classical quantities in terms of these two variables in Cartesian coordinates and then make the component by component substitutions

$$\mathbf{r} \to \text{multiplicative operator } \mathbf{r} \quad \text{and} \quad \mathbf{p} \to \text{differential operator } -i\hbar\nabla. \tag{19.22}$$

This generates the quantum operators corresponding to the classical quantities. For the sake of completeness, we should add that if the classical quantity contains a product of factors whose corresponding operators A and B do not commute, then the operator $\frac{1}{2}(AB + BA)$ is to be substituted for the product.

The substitutions (19.22) invoke operators that are closely connected with the two that we considered at the start of the previous subsection, namely x and $\partial/\partial x$. One, x, corresponds exactly to the x-component of the prescribed quantum position operator; the other, however, has been multiplied by the imaginary constant $-i\hbar$, where $\hbar$ is the Planck constant divided by 2π. This has the (subtle) effect of converting the differential operator into the x-component of an *Hermitian* operator; this is easily verified using integration by parts to show that it satisfies equation (17.16). Without the extra imaginary factor (which changes sign under complex conjugation) the two sides of the equation differ by a minus sign.

Making the differential operator Hermitian does not change in any essential way its commutation properties, and the commutation relation of the two basic quantum operators reads

$$[\,p_x, x\,] = \left[-i\hbar\frac{\partial}{\partial x}, x\right] = -i\hbar. \tag{19.23}$$

Corresponding results hold when x is replaced, in both operators, by y or z. However, it should be noted that if different Cartesian coordinates appear in the two operators then the operators commute, i.e.

$$[\,p_x, y\,] = [\,p_x, z\,] = \left[\,p_y, x\,\right] = \left[\,p_y, z\,\right] = [\,p_z, x\,] = [\,p_z, y\,] = 0. \tag{19.24}$$

As an illustration of the substitution rules, we now construct the Hamiltonian (the quantum-mechanical energy operator) H for a particle of mass m moving in a potential $V(x, y, z)$ when it has one of its allowed energy values, i.e its energy is E_n, where $H|\psi_n\rangle = E_n|\psi_n\rangle$. This latter equation when expressed in a particular coordinate system is the Schrödinger equation for the particle. In terms of position and momentum, the total classical energy of the particle is given by

$$E = \frac{p^2}{2m} + V(x, y, z) = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x, y, z).$$

Substituting $-i\hbar\partial/\partial x$ for p_x (and similarly for p_y and p_z) in the first term on the

RHS gives

$$\frac{(-i\hbar)^2}{2m}\frac{\partial}{\partial x}\frac{\partial}{\partial x}+\frac{(-i\hbar)^2}{2m}\frac{\partial}{\partial y}\frac{\partial}{\partial y}+\frac{(-i\hbar)^2}{2m}\frac{\partial}{\partial z}\frac{\partial}{\partial z}.$$

The potential energy V, being a function of position only, becomes a purely multiplicative operator, thus creating the full expression for the Hamiltonian,

$$H=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(x,y,z),$$

and giving the corresponding Schrödinger equation as

$$H\psi_n=-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi_n}{\partial x^2}+\frac{\partial^2\psi_n}{\partial y^2}+\frac{\partial^2\psi_n}{\partial z^2}\right)+V(x,y,z)\psi_n=E_n\psi_n.$$

We are not so much concerned in this section with solving such differential equations, but with the commutation properties of the operators from which they are constructed. To this end, we now turn our attention to the topic of angular momentum, the operators for which can be constructed in a straightforward manner from the two basic sets.

19.2.1 Angular momentum operators

As required by the substitution rules, we start by expressing angular momentum in terms of the classical quantities $\mathbf{r}$ and $\mathbf{p}$, namely $\mathbf{L}=\mathbf{r}\times\mathbf{p}$ with Cartesian components

$$L_z=xp_y-yp_x,\quad L_x=yp_z-zp_y,\quad L_y=zp_x-xp_z.$$

Making the substitutions (19.22) yields as the corresponding quantum-mechanical operators

$$\begin{aligned}L_z&=-i\hbar\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right),\\ L_x&=-i\hbar\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right),\\ L_y&=-i\hbar\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right).\end{aligned}\tag{19.25}$$

It should be noted that for xp_y, say, x and $\partial/\partial y$ commute, and there is no ambiguity about the way it is to be carried into its quantum form. Further, since the operators corresponding to each of its factors commute and are Hermitian, the operator corresponding to the product is Hermitian. This was shown directly for matrices in exercise 8.7, and can be verified using equation (17.16).

The first question that arises is whether or not these three operators commute.

Consider first

$$L_xL_y = -\hbar^2\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$
$$= -\hbar^2\left(y\frac{\partial}{\partial x} + yz\frac{\partial^2}{\partial z\partial x} - yx\frac{\partial^2}{\partial z^2} - z^2\frac{\partial^2}{\partial y\partial x} + zx\frac{\partial^2}{\partial y\partial z}\right).$$

Now consider

$$L_yL_x = -\hbar^2\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$
$$= -\hbar^2\left(zy\frac{\partial^2}{\partial x\partial z} - z^2\frac{\partial^2}{\partial x\partial y} - xy\frac{\partial^2}{\partial z^2} + x\frac{\partial}{\partial y} + xz\frac{\partial^2}{\partial z\partial y}\right).$$

These two expressions are *not* the same. The difference between them, i.e. the commutator of L_x and L_y, is given by

$$\left[L_x, L_y\right] = L_xL_y - L_yL_x = \hbar^2\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = i\hbar L_z. \qquad (19.26)$$

This, and two similar results obtained by permutting x, y and z cyclically, summarise the commutation relationships between the quantum operators corresponding to the three Cartesian components of angular momentum:

$$\begin{aligned}\left[L_x, L_y\right] &= i\hbar L_z,\\ \left[L_y, L_z\right] &= i\hbar L_x,\\ \left[L_z, L_x\right] &= i\hbar L_y.\end{aligned} \qquad (19.27)$$

As well as its separate components of angular momentum, the total angular momentum associated with a particular state $|\psi\rangle$ is a physical quantity of interest. This is measured by the operator corresponding to the sum of squares of its components,

$$L^2 = L_x^2 + L_y^2 + L_z^2. \qquad (19.28)$$

This is an Hermitian operator, as each term in it is the product of two Hermitian operators that (trivially) commute. It might seem natural to want to 'take the square root' of this operator, but such a process is undefined and we will not pursue the matter.

We next show that, although no two of its components commute, the total angular momentum operator does commute with each of its components. In the proof we use some of the properties (19.17) to (19.20) and result (19.27). We begin with

$$\begin{aligned}
\left[L^2, L_z\right] &= \left[L_x^2 + L_y^2 + L_z^2, L_z\right] \\
&= L_x\left[L_x, L_z\right] + \left[L_x, L_z\right] L_x \\
&\qquad + L_y\left[L_y, L_z\right] + \left[L_y, L_z\right] L_y + \left[L_z^2, L_z\right] \\
&= L_x(-i\hbar)L_y + (-i\hbar)L_y L_x + L_y(i\hbar)L_x + (i\hbar)L_x L_y + 0 \\
&= 0.
\end{aligned}$$

Thus operators L^2 and L_z commute and, continuing in the same way, it can be shown that

$$\left[L^2, L_x\right] = \left[L^2, L_y\right] = \left[L^2, L_z\right] = 0. \tag{19.29}$$

Eigenvalues of the angular momentum operators

We will now use the commutation relations for L^2 and its components to find the eigenvalues of L^2 and L_z, without reference to any specific wavefunction. In other words, the eigenvalues of the operators follow from the structure of their commutators. There is nothing particular about L_z, and L_x or L_y could equally well have been chosen, though, in general, it is not possible to find states that are simultaneously eigenstates of two or more of L_x, L_y and L_z.

To help with the calculation, it is convenient to define the two operators

$$U \equiv L_x + iL_y \quad \text{and} \quad D \equiv L_x - iL_y.$$

These operators are not Hermitian; they are in fact Hermitian conjugates, in that $U^\dagger = D$ and $D^\dagger = U$, but they do not represent measurable physical quantities. We first note their multiplication and commutation properties:

$$\begin{aligned}
UD &= (L_x + iL_y)(L_x - iL_y) = L_x^2 + L_y^2 + i\left[L_y, L_x\right] \\
&= L^2 - L_z^2 + \hbar L_z, && (19.30)\\
DU &= (L_x - iL_y)(L_x + iL_y) = L_x^2 + L_y^2 - i\left[L_y, L_x\right] \\
&= L^2 - L_z^2 - \hbar L_z, && (19.31)\\
\left[L_z, U\right] &= \left[L_z, L_x\right] + i\left[L_z, L_y\right] = i\hbar L_y + \hbar L_x = \hbar U, && (19.32)\\
\left[L_z, D\right] &= \left[L_z, L_x\right] - i\left[L_z, L_y\right] = i\hbar L_y - \hbar L_x = -\hbar D. && (19.33)
\end{aligned}$$

In the same way as was shown for matrices, it can be demonstrated that if two operators commute they have a common set of eigenstates. Since L^2 and L_z commute they possess such a set; let one of the set be $|\psi\rangle$ with

$$L^2|\psi\rangle = a|\psi\rangle \quad \text{and} \quad L_z|\psi\rangle = b|\psi\rangle.$$

Now consider the state $|\psi'\rangle = U|\psi\rangle$ and the actions of L^2 and L_z upon it.

Consider first $L^2|\psi'\rangle$, recalling that L^2 commutes with both L_x and L_y and hence with U:

$$L^2|\psi'\rangle = L^2U|\psi\rangle = UL^2|\psi\rangle = Ua|\psi\rangle = aU|\psi\rangle = a|\psi'\rangle.$$

Thus, $|\psi'\rangle$ is also an eigenstate of L^2, corresponding to the same eigenvalue as $|\psi\rangle$. Now consider the action of L_z:

$$\begin{aligned} L_z|\psi'\rangle &= L_zU|\psi\rangle \\ &= (UL_z + \hbar U)|\psi\rangle, \text{ using } [L_z, U] = \hbar U, \\ &= Ub|\psi\rangle + \hbar U|\psi\rangle \\ &= (b+\hbar)U|\psi\rangle \\ &= (b+\hbar)|\psi'\rangle. \end{aligned}$$

Thus, $|\psi'\rangle$ is also an eigenstate of L_z, but with eigenvalue $b+\hbar$.

In summary, the effect of U acting upon $|\psi\rangle$ is to produce a new state that has the same eigenvalue for L^2 and is still an eigenstate of L_z, though with that eigenvalue increased by $\hbar$. An exactly analogous calculation shows that the effect of D acting upon $|\psi\rangle$ is to produce another new state, one that also has the same eigenvalue for L^2 and is also still an eigenstate of L_z, though with the eigenvalue decreased by $\hbar$ in this case. For these reasons, U and D are usually known as *ladder* operators.

It is clear that, by starting from any arbitrary eigenstate and repeatedly applying either U or D, we could generate a series of eigenstates, all of which have the eigenvalue a for L^2, but increment in their L_z eigenvalues by $\pm\hbar$. However, we also have the physical requirement that, for real values of the z-component, its square cannot exceed the square of the total angular momentum, i.e. $b^2 \le a$. Thus b has a maximum value c that satisfies

$$c^2 \le a \quad \text{but} \quad (c+\hbar)^2 > a;$$

let the corresponding eigenstate be $|\psi_u\rangle$ with $L_z|\psi_u\rangle = c|\psi_u\rangle$. Now it is still true that

$$L_zU|\psi_u\rangle = (c+\hbar)U|\psi_u\rangle,$$

and, to make this compatible with the physical constraint, we must have that $U|\psi_u\rangle$ is the zero ket vector $|\,\emptyset\,\rangle$. Now, using result (19.31), we have

$$\begin{aligned} DU|\psi_u\rangle &= (L^2 - L_z^2 - \hbar L_z)|\psi_u\rangle, \\ \Rightarrow \quad 0|\,\emptyset\,\rangle = D|\,\emptyset\,\rangle &= (a^2 - c^2 - \hbar c)|\psi_u\rangle, \\ \Rightarrow \quad a &= c(c+\hbar). \end{aligned}$$

This gives the relationship between a and c. We now establish the possible forms for c.

If we start with eigenstate $|\psi_u\rangle$, which has the highest eigenvalue c for L_z, and operate repeatedly on it with the (down) ladder operator D, we will generate a state $|\psi_d\rangle$ which, whilst still an eigenstate of L^2 with eigenvalue a, has the lowest physically possible value, d say, for the eigenvalue of L_z. If this happens after n operations we will have that $d = c - n\hbar$ and

$$L_z|\psi_d\rangle = (c - n\hbar)|\psi_d\rangle.$$

Arguing in the same way as previously that $D|\psi_d\rangle$ must be an unphysical ket vector, we conclude that

$$\begin{aligned}
0|\,\emptyset\,\rangle = U|\,\emptyset\,\rangle &= UD|\psi_d\rangle \\
&= (L^2 - L_z^2 + \hbar L_z)|\psi_d\rangle, \text{ using (19.30)}, \\
&= [\,a - (c - n\hbar)^2 + \hbar(c - n\hbar)\,]|\psi_d\rangle \\
\Rightarrow \quad a &= (c - n\hbar)^2 - \hbar(c - n\hbar).
\end{aligned}$$

Equating the two results for a gives

$$\begin{aligned}
c^2 + c\hbar &= c^2 - 2cn\hbar + n^2\hbar^2 - c\hbar + n\hbar^2, \\
2c(n+1) &= n(n+1)\hbar, \\
c &= \tfrac{1}{2}n\hbar.
\end{aligned}$$

Since n is necessarily integral, c is an integer multiple of $\frac{1}{2}\hbar$. This result is valid irrespective of which eigenstate $|\psi\rangle$ we started with, though the actual value of the integer n depends on $|\psi_u\rangle$ and hence upon $|\psi\rangle$.

Denoting $\frac{1}{2}n$ by ℓ we can say that the possible eigenvalues of the operator L_z, and hence the possible results of a measurement of the z-component of the angular momentum of a system, are given by

$$\ell\hbar, \quad (\ell - 1)\hbar, \quad (\ell - 2)\hbar, \quad \ldots, \quad -\ell\hbar.$$

The value of a for all $2\ell + 1$ of the corresponding states,

$$|\psi_u\rangle, \quad D|\psi_u\rangle, \quad D^2|\psi_u\rangle, \quad \ldots, \quad D^{2\ell}|\psi_u\rangle,$$

is $\ell(\ell + 1)\hbar^2$.

The similarity of form between this eigenvalue and that appearing in Legendre's equation is not an accident. It is intimately connected with the facts (i) that L^2 is a measure of the rotational kinetic energy of a particle in a system centred on the origin, and (ii) that in spherical polar coordinates L^2 has the same form as the angle-dependent part of ∇^2, which, as we have seen, is itself proportional to the quantum-mechanical kinetic energy operator. Legendre's equation and the associated Legendre equation arise naturally when $\nabla^2\psi = f(r)$ is solved in spherical polar coordinates using the method of separation of variables discussed in chapter 21.

The derivation of the eigenvalues $\ell(\ell+1)\hbar^2$ and $m\hbar$, with $-\ell \le m \le \ell$, depends only on the commutation relationships between the corresponding operators. Any other set of four operators with the same commutation structure would result in the same eigenvalue spectrum. In fact, quantum mechanically, orbital angular momentum is restricted to cases in which n is even and so ℓ is an integer; this is in accord with the requirement placed on ℓ if solutions to $\nabla^2\psi = f(r)$ that are finite on the polar axis are to be obtained. The non-classical notion of internal angular momentum (spin) for a particle provides a set of operators that are able to take both integral and half-integral multiples of $\hbar$ as their eigenvalues.

We have already seen that, for a state $|\ell, m\rangle$ that has a z-component of angular momentum $m\hbar$, the state $U|\ell, m\rangle$ is one with its z-component of angular momentum equal to $(m+1)\hbar$. But the new state ket vector so produced is not necessarily normalised so as to make $\langle \ell, m+1 \,|\, \ell, m+1\rangle = 1$. We will conclude this discussion of angular momentum by calculating the coefficients μ_m and ν_m in the equations

$$U|\ell, m\rangle = \mu_m|\ell, m+1\rangle \quad \text{and} \quad D|\ell, m\rangle = \nu_m|\ell, m-1\rangle$$

on the basis that $\langle \ell, r \,|\, \ell, r\rangle = 1$ for all ℓ and r.

To do so, we consider the inner product $I = \langle \ell, m \,|DU|\, \ell, m\rangle$, evaluated in two different ways. We have already noted that U and D are Hermitian conjugates and so I can be written as

$$I = \langle \ell, m \,|U^\dagger U|\, \ell, m\rangle = \mu_m^*\langle \ell, m \,|\, \ell, m\rangle\mu_m = |\mu_m|^2.$$

But, using equation (19.31), it can also be expressed as

$$\begin{aligned} I &= \langle \ell, m \,|L^2 - L_z^2 - \hbar L_z|\, \ell, m\rangle \\ &= \langle \ell, m \,|\ell(\ell+1)\hbar^2 - m^2\hbar^2 - m\hbar^2|\, \ell, m\rangle \\ &= [\,\ell(\ell+1)\hbar^2 - m^2\hbar^2 - m\hbar^2\,]\,\langle \ell, m \,|\, \ell, m\rangle \\ &= [\,\ell(\ell+1) - m(m+1)\,]\,\hbar^2. \end{aligned}$$

Thus we are required to have

$$|\mu_m|^2 = [\,\ell(\ell+1) - m(m+1)\,]\,\hbar^2,$$

but can choose that all μ_m are real and non-negative (recall that $|m| \leq \ell$). A similar calculation can be used to calculate ν_m. The results are summarised in the equations

$$U|\,\ell, m\rangle = \sqrt{\ell(\ell+1) - m(m+1)}\,\hbar|\,\ell, m+1\rangle, \tag{19.34}$$

$$D|\,\ell, m\rangle = \sqrt{\ell(\ell+1) - m(m-1)}\,\hbar|\,\ell, m-1\rangle. \tag{19.35}$$

It can easily be checked that $U|\ell, \ell\rangle = |\,\emptyset\,\rangle = D|\ell, -\ell\rangle$.

19.2.2 Uncertainty principles

The next topic we explore is the quantitative consequences of a non-zero commutator for two quantum (Hermitian) operators that correspond to physical variables.

As previously noted, the expectation value in a state $|\psi\rangle$ of the physical quantity A corresponding to the operator A is $E[A] = \langle\psi|\, A\,|\psi\rangle$. Any one measurement of A can only yield one of the eigenvalues of A. But if repeated measurements could be made on a large number of identical systems, a discrete or continuous range of values would be obtained. It is a natural extension of normal data analysis to measure the uncertainty in the value of A by the observed variance in the measured values of A, denoted by $(\Delta A)^2$ and calculated as the average value of $(A - E[A])^2$. The expected value of this variance for the state $|\psi\rangle$ is given by $\langle\psi\,|(A - E[A]\,)^2|\psi\rangle$.

We now give a mathematical proof that there is a theoretical lower limit for the product of the uncertainties in any two physical quantities, and we start by proving a result similar to the Schwarz inequality. Let $|u\rangle$ and $|v\rangle$ be any two state vectors and let λ be any *real* scalar. Then consider the vector $|w\rangle = |u\rangle + \lambda|v\rangle$ and, in particular, note that

$$0 \le \langle w\,|\,w\rangle = \langle u\,|\,u\rangle + \lambda(\langle u\,|\,v\rangle + \langle v\,|\,u\rangle) + \lambda^2\langle v\,|\,v\rangle.$$

This is a quadratic inequality in λ and therefore the quadratic equation formed by equating the RHS to zero must have no real roots. The coefficient of λ is $(\langle u\,|\,v\rangle + \langle v\,|\,u\rangle) = 2\,\mathrm{Re}\,\langle u\,|\,v\rangle$ and its square is thus ≥ 0. The condition for no real roots of the quadratic is therefore

$$0 \le (\langle u\,|\,v\rangle + \langle v\,|\,u\rangle)^2 \le 4\langle u\,|\,u\rangle\,\langle v\,|\,v\rangle. \tag{19.36}$$

This result will now be applied to state vectors constructed from $|\psi\rangle$, the state vector of the particular system for which we wish to establish a relationship between the uncertainties in the two physical variables corresponding to (Hermitian) operators A and B. We take

$$|u\rangle = (A - E[A])\,|\,\psi\rangle \quad \text{and} \quad |v\rangle = i(B - E[B])\,|\,\psi\rangle. \tag{19.37}$$

Then

$$\langle u\,|\,u\rangle = \langle\psi\,|(A - E[A]\,)^2|\psi\rangle = (\Delta A)^2,$$
$$\langle v\,|\,v\rangle = \langle\psi\,|(B - E[B]\,)^2|\psi\rangle = (\Delta B)^2.$$

Further,

$$\begin{aligned}\langle u\,|\,v\rangle &= \langle\psi\,|\,(A - E[A])i(B - E[B])\,|\,\psi\rangle \\ &= i\langle\psi\,|\,AB\,|\,\psi\rangle - iE[A]\langle\psi\,|\,B\,|\,\psi\rangle - iE[B]\langle\psi\,|\,A\,|\,\psi\rangle + iE[A]E[B]\langle\psi\,|\,\psi\rangle \\ &= i\langle\psi\,|\,AB\,|\,\psi\rangle - iE[A]E[B].\end{aligned}$$

In the second line, we have moved expectation values, which are purely numbers, out of the inner products and used the normalisation condition $\langle\psi|\psi\rangle = 1$. Similarly

$$\langle v \,|\, u\rangle = -i\langle\psi \,|\, BA \,|\, \psi\rangle + iE[A]E[B].$$

Adding these two results gives

$$\langle u \,|\, v\rangle + \langle v \,|\, u\rangle = i\langle\psi \,|\, AB - BA \,|\psi\rangle,$$

and substitution into (19.36) yields

$$0 \leq (i\langle\psi \,|\, AB - BA \,|\psi\rangle)^2 \leq 4(\Delta A)^2(\Delta B)^2$$

At first sight, the middle term of this inequality might appear to be negative, but this is not so. Since A and B are Hermitian, $AB - BA$ is anti-Hermitian, as is easily demonstrated. Since i is also anti-Hermitian, the quantity in the parentheses in the middle term is real and its square non-negative. Rearranging the equation and expressing it in terms of the commutator of A and B gives the generalised form of the *Uncertainty Principle*. For any particular state $|\psi\rangle$ of a system, this provides the quantitative relationship between the minimum value that the product of the uncertainties in A and B can have and the expectation value, in that state, of their commutator,

$$(\Delta A)^2(\Delta B)^2 \geq \tfrac{1}{4}|\,\langle\psi \,|\, [\,A, B\,] \,|\, \psi\rangle\,|^2. \tag{19.38}$$

Immediate observations include the following:

(i) If A and B commute there is no absolute restriction on the accuracy with which the corresponding physical quantities may be known. That is not to say that ΔA and ΔB will always be zero, only that they may be.
(ii) If the commutator of A and B is a constant, $k \neq 0$, then the RHS of equation (19.38) is necessarily equal to $\frac{1}{4}|k|^2$, whatever the form of $|\psi\rangle$, and it is not possible to have $\Delta A = \Delta B = 0$.
(iii) Since the RHS depends upon $|\psi\rangle$, it is possible, even for two operators that do not commute, for the lower limit of $(\Delta A)^2(\Delta B)^2$ to be zero. This will occur if the commutator $[\,A, B\,]$ is itself an operator whose expectation value in the particular state $|\psi\rangle$ happens to be zero.

To illustrate the third of these, we might consider the components of angular momentum discussed in the previous subsection. There, in equation (19.27), we found that the commutator of the operators corresponding to the x- and y-components of angular momentum is non-zero; in fact, it has the value $i\hbar L_z$. This means that if the state $|\psi\rangle$ of a system happened to be such that $\langle\psi|L_z|\psi\rangle = 0$, as it would if, for example, it were the eigenstate of L_z, $|\psi\rangle = |\ell, 0\rangle$, then there would be no fundamental reason why the physical values of both L_x and L_y should not be known exactly. Indeed, if the state were spherically symmetric, and hence formally an eigenstate of L^2 with $\ell = 0$, all three components of angular momentum could be (and are) known to be zero.

►*Working in one dimension, show that the minimum value of the product $\Delta p_x \times \Delta x$ for a particle is $\frac{1}{2}\hbar$. Find the form of the wavefunction that attains this minimum value for a particle whose expectation values for position and momentum are $\bar{x}$ and $\bar{p}$, respectively.*

We have already seen, in (19.23) that the commutator of p_x and x is $-i\hbar$, a constant. Therefore, irrespective of the actual form of $|\psi\rangle$, the RHS of (19.38) is $\frac{1}{4}\hbar^2$ (see observation (ii) above). Thus, since all quantities are positive, taking the square roots of both sides of the equation shows directly that

$$\Delta p_x \times \Delta x \geq \tfrac{1}{2}\hbar.$$

Returning to the derivation of the Uncertainty Principle, we see that the inequality becomes an equality only when

$$(\langle u \,|\, v\rangle + \langle v \,|\, u\rangle)^2 = 4\langle u \,|\, u\rangle \, \langle v \,|\, v\rangle.$$

The RHS of this equality has the value $4||u||^2||v||^2$ and so, by virtue of Schwarz's inequality, we have

$$\begin{aligned}
4\|u\|^2\|v\|^2 &= (\langle u \,|\, v\rangle + \langle v \,|\, u\rangle)^2 \\
&\leq (|\langle u \,|\, v\rangle| + |\langle v \,|\, u\rangle|)^2 \\
&\leq (\|u\| \, \|v\| + \|v\| \, \|u\|)^2 \\
&= 4\|u\|^2\|v\|^2.
\end{aligned}$$

Since the LHS is less than or equal to something that has the same value as itself, all of the inequalities are, in fact, equalities. Thus $\langle u|v\rangle = \|u\| \, \|v\|$, showing that $|u\rangle$ and $|v\rangle$ are parallel vectors, i.e. $|u\rangle = \mu|v\rangle$ for some scalar μ.

We now transform this condition into a constraint that the wavefunction $\psi = \psi(x)$ must satisfy. Recalling the definitions (19.37) of $|u\rangle$ and $|v\rangle$ in terms of $|\psi\rangle$, we have

$$\left(-i\hbar\frac{d}{dx} - \bar{p}\right)\psi = \mu i(x - \bar{x})\psi,$$

$$\frac{d\psi}{dx} + \frac{1}{\hbar}[\,\mu(x - \bar{x}) - i\bar{p}\,]\psi = 0.$$

The IF for this equation is $\exp\left[\dfrac{\mu(x-\bar{x})^2}{2\hbar} - \dfrac{i\bar{p}x}{\hbar}\right]$, giving

$$\frac{d}{dx}\left\{\psi \, \exp\left[\frac{\mu(x-\bar{x})^2}{2\hbar} - \frac{i\bar{p}x}{\hbar}\right]\right\} = 0,$$

which, in turn, leads to

$$\psi(x) = A\exp\left[-\frac{\mu(x-\bar{x})^2}{2\hbar}\right] \exp\left(\frac{i\bar{p}x}{\hbar}\right).$$

From this it is apparent that the minimum uncertainty product $\Delta p_x \times \Delta x$ is obtained when the probability density $|\psi(x)|^2$ has the form of a Gaussian distribution centred on $\bar{x}$. The value of μ is not fixed by this consideration and it could be anything (positive); a large value for μ would yield a small value for Δx but a correspondingly large one for Δp_x. ◄

19.2.3 Annihilation and creation operators

As a final illustration of the use of operator methods in physics we consider their application to the quantum mechanics of a simple harmonic oscillator (s.h.o.). Although we will start with the conventional description of a one-dimensional oscillator, using its position and momentum, we will recast the description in terms of two operators and their commutator and show that many important conclusions can be reached from studying these alone.

The Hamiltonian for a particle of mass m with momentum p moving in a one-dimensional parabolic potential $V(x) = \frac{1}{2}kx^2$ is

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2,$$

where its classical frequency of oscillation ω is given by $\omega^2 = k/m$. We recall that the corresponding operators, p and x, do not commute and that $[\,p, x\,] = -i\hbar$.

In analogy with the ladder operators used when discussing angular momentum, we define two new operators:

$$A \equiv \sqrt{\frac{m\omega}{2}}\,x + \frac{ip}{\sqrt{2m\omega}} \quad \text{and} \quad A^\dagger \equiv \sqrt{\frac{m\omega}{2}}\,x - \frac{ip}{\sqrt{2m\omega}}. \tag{19.39}$$

Since both x and p are Hermitian, A and $A^\dagger$ are Hermitian conjugates, though neither is Hermitian and they do not represent physical quantities that can be measured.

Now consider the two products $A^\dagger A$ and $AA^\dagger$:

$$A^\dagger A = \frac{m\omega}{2}x^2 - \frac{ipx}{2} + \frac{ixp}{2} + \frac{p^2}{2m\omega} = \frac{H}{\omega} - \frac{i}{2}[\,p, x\,] = \frac{H}{\omega} - \frac{\hbar}{2},$$

$$AA^\dagger = \frac{m\omega}{2}x^2 + \frac{ipx}{2} - \frac{ixp}{2} + \frac{p^2}{2m\omega} = \frac{H}{\omega} + \frac{i}{2}[\,p, x\,] = \frac{H}{\omega} + \frac{\hbar}{2}.$$

From these it follows that

$$H = \tfrac{1}{2}\omega(A^\dagger A + AA^\dagger) \tag{19.40}$$

and that

$$\left[A, A^\dagger\right] = \hbar. \tag{19.41}$$

Further,

$$\begin{aligned}[\,H, A\,] &= \left[\tfrac{1}{2}\omega(A^\dagger A + AA^\dagger), A\right] \\ &= \tfrac{1}{2}\omega\left(A^\dagger\, 0 + \left[A^\dagger, A\right]A + A\left[A^\dagger, A\right] + 0\, A^\dagger\right) \\ &= \tfrac{1}{2}\omega(-\hbar A - A\hbar) = -\hbar\omega A. \end{aligned} \tag{19.42}$$

Similarly,

$$\left[H, A^\dagger\right] = \hbar\omega A^\dagger \tag{19.43}$$

Before we apply these relationships to the question of the energy spectrum of the s.h.o., we need to prove one further result. This is that if B is an Hermitian operator then $\langle\psi\,|\,B^2\,|\,\psi\rangle \geq 0$ for *any* $|\psi\rangle$. The proof, which involves introducing an arbitrary complete set of orthonormal base states $|\phi_i\rangle$ and using equation (19.11), is as follows:

$$\begin{aligned}
\langle\psi\,|\,B^2\,|\,\psi\rangle &= \langle\psi\,|\,B\times 1\ \times B\,|\,\psi\,\rangle \\
&= \sum_i \langle\psi\,|\,B\,|\phi_i\rangle\langle\phi_i\,|\,B\,|\psi\rangle \\
&= \sum_i \langle\psi\,|\,B\,|\phi_i\rangle\left(\langle\phi_i\,|\,B\,|\psi\rangle^*\right)^* \\
&= \sum_i \langle\psi\,|\,B\,|\phi_i\rangle\left(\langle\psi\,|\,B^\dagger\,|\phi_i\rangle\right)^* \\
&= \sum_i \langle\psi\,|\,B\,|\phi_i\rangle\langle\psi\,|\,B\,|\phi_i\rangle^*, \qquad \text{since } B \text{ is Hermitian,} \\
&= \sum_i |\,\langle\psi\,|\,B\,|\phi_i\rangle\,|^2 \geq 0.
\end{aligned}$$

We note, for future reference, that the Hamiltonian H for the s.h.o. is the sum of two terms each of this form and therefore conclude that $\langle\psi|H|\psi\rangle \geq 0$ for all $|\psi\rangle$.

The energy spectrum of the simple harmonic oscillator

Let the normalised ket vector $|n\rangle$ (or $|E_n\rangle$) denote the nth energy state of the s.h.o. with energy E_n. Then it must be an eigenstate of the (Hermitian) Hamiltonian H and satisfy

$$H|n\rangle = E_n|n\rangle \text{ with } \langle m|n\rangle = \delta_{mn}.$$

Now consider the state $A|n\rangle$ and the effect of H upon it:

$$\begin{aligned}
HA|n\rangle &= AH|n\rangle - \hbar\omega A|n\rangle, \qquad \text{using (19.42),} \\
&= AE_n|n\rangle - \hbar\omega A|n\rangle \\
&= (E_n - \hbar\omega)A|n\rangle.
\end{aligned}$$

Thus $A|n\rangle$ is an eigenstate of H corresponding to energy $E_n - \hbar\omega$ and must be some multiple of the normalised ket vector $|E_n - \hbar\omega\rangle$, i.e.

$$A|\,E_n\rangle \equiv A|n\rangle = c_n|E_n - \hbar\omega\rangle,$$

where c_n is not necessarily of unit modulus. Clearly, A is an operator that generates a new state that is lower in energy by $\hbar\omega$; it can thus be compared to the operator D, which has a similar effect in the context of the z-component of angular momentum. Because it possesses the property of reducing the energy of the state by $\hbar\omega$, which, as we will see, is one quantum of excitation energy for the oscillator, the operator A is called an *annihilation operator*. Repeated application of A, m times say, will produce a state whose energy is $m\hbar\omega$ lower than that of the original:

$$A^m|E_n\rangle = c_n c_{n-1}\cdots c_{n-m+1}|E_n - m\hbar\omega\rangle. \qquad (19.44)$$

In a similar way it can be shown that $A^\dagger$ parallels the operator U of our angular momentum discussion and creates an additional quantum of energy each time it is applied:

$$(A^\dagger)^m|E_n\rangle = d_n d_{n+1}\cdots d_{n+m-1}|E_n + m\hbar\omega\rangle. \tag{19.45}$$

It is therefore known as a *creation operator*.

As noted earlier, the expectation value of the oscillator's energy operator $\langle\psi|H|\psi\rangle$ must be non-negative, and therefore it must have a lowest value. Let this be E_0, with corresponding eigenstate $|0\rangle$. Since the energy-lowering property of A applies to any eigenstate of H, in order to avoid a contradiction we must have that $A|0\rangle = |\,\emptyset\,\rangle$. It then follows from (19.40) that

$$\begin{aligned} H|0\rangle &= \tfrac{1}{2}\omega(A^\dagger A + AA^\dagger)|0\rangle \\ &= \tfrac{1}{2}\omega A^\dagger A|0\rangle + \tfrac{1}{2}\omega(A^\dagger A + \hbar)|0\rangle, \qquad \text{using (19.41)}, \\ &= 0 + 0 + \tfrac{1}{2}\hbar\omega|0\rangle. \end{aligned} \tag{19.46}$$

This shows that the commutator structure of the operators and the form of the Hamiltonian imply that the lowest energy (its ground-state energy) is $\frac{1}{2}\hbar\omega$; this is a result that has been derived without explicit reference to the corresponding wavefunction. This non-zero lowest value for the energy, known as the zero-point energy of the oscillator, and the discrete values for the allowed energy states are quantum-mechanical in origin; classically such an oscillator could have any non-negative energy, including zero.

Working back from this result, we see that the energy levels of the s.h.o. are $\frac{1}{2}\hbar\omega,\ \frac{3}{2}\hbar\omega,\ \frac{5}{2}\hbar\omega,\ldots,(m+\frac{1}{2})\hbar\omega,\ldots$, and that the corresponding (unnormalised) ket vectors can be written as

$$|0\rangle, \qquad A^\dagger|0\rangle, \qquad (A^\dagger)^2|0\rangle, \qquad \ldots, \qquad (A^\dagger)^m|0\rangle, \qquad \ldots.$$

This notation, and elaborations of it, are often used in the quantum treatment of classical fields such as the electromagnetic field. Thus, as the reader should verify, $A(A^\dagger)^3A^2A^\dagger A(A^\dagger)^4|0\rangle$ is a state with energy $\frac{9}{2}\hbar\omega$, whilst $A(A^\dagger)^3A^5A^\dagger A(A^\dagger)^4|0\rangle$ is not a physical state at all.

The normalisation of the eigenstates

In order to make quantitative calculations using the previous results we need to establish the values of the c_n and d_n that appear in equations (19.44) and (19.45). To do this, we first establish the operator recurrence relation

$$A^m(A^\dagger)^m = A^{m-1}(A^\dagger)^m A + m\hbar A^{m-1}(A^\dagger)^{m-1}. \tag{19.47}$$

The proof, which makes repeated use of $\left[A, A^\dagger\right] = \hbar$, is as follows:

$$\begin{aligned}
A^m(A^\dagger)^m &= A^{m-1}AA^\dagger(A^\dagger)^{m-1} \\
&= A^{m-1}(A^\dagger A + \hbar)(A^\dagger)^{m-1} \\
&= A^{m-1}A^\dagger A(A^\dagger)^{m-1} + \hbar A^{m-1}(A^\dagger)^{m-1} \\
&= A^{m-1}A^\dagger(A^\dagger A + \hbar)(A^\dagger)^{m-2} + \hbar A^{m-1}(A^\dagger)^{m-1} \\
&= A^{m-1}(A^\dagger)^2 A(A^\dagger)^{m-2} + A^{m-1}A^\dagger\hbar(A^\dagger)^{m-2} + \hbar A^{m-1}(A^\dagger)^{m-1} \\
&= A^{m-1}(A^\dagger)^2(A^\dagger A + \hbar)(A^\dagger)^{m-3} + 2\hbar A^{m-1}(A^\dagger)^{m-1} \\
&\ \vdots \\
&= A^{m-1}(A^\dagger)^m A + m\hbar A^{m-1}(A^\dagger)^{m-1}.
\end{aligned}$$

Now we take the expectation values in the ground state $|0\rangle$ of both sides of this operator equation and note that the first term on the RHS is zero since it contains the term $A|0\rangle$. The non-vanishing terms are

$$\langle 0 \,|\, A^m(A^\dagger)^m \,|\, 0\rangle = m\hbar\langle 0 \,|\, A^{m-1}(A^\dagger)^{m-1} \,|\, 0\rangle.$$

The LHS is the square of the norm of $(A^\dagger)^m|0\rangle$, and, from equation (19.45), it is equal to

$$|d_0|^2|d_1|^2 \cdots |d_{m-1}|^2 \,\langle 0 \,|\, 0\rangle.$$

Similarly, the RHS is equal to

$$m\hbar\,|d_0|^2|d_1|^2 \cdots |d_{m-2}|^2 \,\langle 0 \,|\, 0\rangle.$$

It follows that $|d_{m-1}|^2 = m\hbar$ and, taking all coefficients as real, $d_m = \sqrt{(m+1)\hbar}$. Thus the correctly normalised state of energy $(n + \frac{1}{2})\hbar$, obtained by repeated application of $A^\dagger$ to the ground state, is given by

$$|n\rangle = \frac{(A^\dagger)^n}{(n!\,\hbar^n)^{1/2}}\,|0\rangle. \tag{19.48}$$

To evaluate the c_n, we note that, from the commutator of A and $A^\dagger$,

$$\begin{aligned}
\left[A, A^\dagger\right]\,|n\rangle &= AA^\dagger|n\rangle - A^\dagger A|n\rangle \\
\hbar\,|n\rangle &= \sqrt{(n+1)\hbar}\,A\,|n+1\rangle - c_n\,A^\dagger\,|n-1\rangle \\
&= \sqrt{(n+1)\hbar}\,c_{n+1}\,|n\rangle - c_n\sqrt{n\hbar}\,|n\rangle, \\
\hbar &= \sqrt{(n+1)\hbar}\,c_{n+1} - c_n\sqrt{n\hbar},
\end{aligned}$$

which has the obvious solution $c_n = \sqrt{n\hbar}$. To summarise:

$$c_n = \sqrt{n\hbar} \qquad \text{and} \qquad d_n = \sqrt{(n+1)\hbar}. \tag{19.49}$$

We end this chapter with another worked example. This one illustrates how the operator formalism that we have developed can be used to obtain results that would involve a number of non-trivial integrals if tackled using explicit wavefunctions.

►*Given that the first-order change in the ground-state energy of a quantum system when it is perturbed by a small additional term H' in the Hamiltonian is $\langle 0|H'|0\rangle$, find the first-order change in the energy of a simple harmonic oscillator in the presence of an additional potential $V'(x) = \lambda x^3 + \mu x^4$.*

From the definitions of A and $A^\dagger$, equation (19.39), we can write

$$x = \frac{1}{\sqrt{2m\omega}}(A + A^\dagger) \quad \Rightarrow \quad H' = \frac{\lambda}{(2m\omega)^{3/2}}(A + A^\dagger)^3 + \frac{\mu}{(2m\omega)^2}(A + A^\dagger)^4.$$

We now compute successive values of $(A + A^\dagger)^n |0\rangle$ for $n = 1, 2, 3, 4$, remembering that

$$A\,|n\rangle = \sqrt{n\hbar}\,|n-1\rangle \qquad \text{and} \qquad A^\dagger\,|n\rangle = \sqrt{(n+1)\hbar}\,|n+1\rangle\ :$$

$$\begin{aligned}
(A + A^\dagger)\,|0\rangle &= 0 + \hbar^{1/2}\,|1\rangle,\\
(A + A^\dagger)^2\,|0\rangle &= \hbar\,|0\rangle + \sqrt{2}\,\hbar\,|2\rangle,\\
(A + A^\dagger)^3\,|0\rangle &= 0 + \hbar^{3/2}\,|1\rangle + 2\hbar^{3/2}\,|1\rangle + \sqrt{6}\,\hbar^{3/2}\,|3\rangle\\
&= 3\hbar^{3/2}\,|1\rangle + \sqrt{6}\,\hbar^{3/2}\,|3\rangle,\\
(A + A^\dagger)^4\,|0\rangle &= 3\hbar^2\,|0\rangle + \sqrt{18}\,\hbar^2\,|2\rangle + \sqrt{18}\,\hbar^2\,|2\rangle + \sqrt{24}\,\hbar^2\,|4\rangle.
\end{aligned}$$

To find the energy shift we need to form the inner product of each of these state vectors with $|0\rangle$. But $|0\rangle$ is orthogonal to all $|n\rangle$ if $n \neq 0$. Consequently, the term $\langle 0|\,(A + A^\dagger)^3\,|0\rangle$ in the expectation value is zero, and in the expression for $\langle 0|\,(A + A^\dagger)^4\,|0\rangle$ only the first term is non-zero; its value is $3\hbar^2$. The perturbation energy is thus given by

$$\langle 0\,|\,H'\,|\,0\rangle = \frac{3\mu\hbar^2}{(2m\omega)^2}.$$

It could have been anticipated on symmetry grounds that the expectation of λx^3, an odd function of x, would be zero, but the calculation gives this result automatically. The contribution of the quadratic term in the perturbation would have been much harder to anticipate! ◄

19.3 Exercises

19.1 Show that the commutator of two operators that correspond to two physical observables cannot itself correspond to another physical observable.

19.2 By expressing the operator L_z, corresponding to the z-component of angular momentum, in spherical polar coordinates (r, θ, ϕ), show that the angular momentum of a particle about the polar axis cannot be known at the same time as its azimuthal position around that axis.

19.3 In quantum mechanics, the time dependence of the state function $|\psi\rangle$ of a system is given, as a further postulate, by the equation

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle,$$

where H is the Hamiltonian of the system. Use this to find the time dependence of the expectation value $\langle A\rangle$ of an operator A that itself has no explicit time dependence. Hence show that operators that commute with the Hamiltonian correspond to the classical 'constants of the motion'.

For a particle of mass m moving in a one-dimensional potential $V(x)$, prove Ehrenfest's theorem:

$$\frac{d\langle p_x\rangle}{dt} = -\left\langle \frac{dV}{dx} \right\rangle \quad \text{and} \quad \frac{d\langle x\rangle}{dt} = \frac{\langle p_x\rangle}{m}.$$

19.4 Show that the Pauli matrices

$$\mathsf{S}_x = \tfrac{1}{2}\hbar\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathsf{S}_y = \tfrac{1}{2}\hbar\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathsf{S}_z = \tfrac{1}{2}\hbar\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

which are used as the operators corresponding to intrinsic spin of $\frac{1}{2}\hbar$ in non-relativistic quantum mechanics, satisfy $\mathsf{S}_x^2 = \mathsf{S}_y^2 = \mathsf{S}_z^2 = \frac{1}{4}\hbar^2\mathsf{I}$, and have the same commutation properties as the components of orbital angular momentum. Deduce that any state $|\psi\rangle$ represented by the column vector $(a,\ b)^{\mathrm{T}}$ is an eigenstate of S^2 with eigenvalue $3\hbar^2/4$.

19.5 Find closed-form expressions for $\cos\mathsf{C}$ and $\sin\mathsf{C}$, where C is the matrix

$$\mathsf{C} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Demonstrate that the 'expected' relationships

$$\cos^2\mathsf{C} + \sin^2\mathsf{C} = \mathsf{I} \quad \text{and} \quad \sin 2\mathsf{C} = 2\sin\mathsf{C}\cos\mathsf{C}$$

are valid.

19.6 Operators A and B anticommute. Evaluate $(A+B)^{2n}$ for a few values of n and hence propose an expression for c_{nr} in the expansion

$$(A+B)^{2n} = \sum_{r=0}^{n} c_{nr}\, A^{2n-2r}\, B^{2r}.$$

Prove your proposed formula for general values of n, using the method of induction.

Show that

$$\cos(A+B) = \sum_{n=0}^{\infty}\sum_{r=0}^{n} d_{nr}\, A^{2n-2r} B^{2r},$$

where the d_{nr} are constants whose values you should determine.

By taking as A the matrix $\mathsf{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, confirm that your answer is consistent with that obtained in exercise 19.5.

19.7 Expressed in terms of the annihilation and creation operators A and $A^\dagger$ discussed in the text, a system has an unperturbed Hamiltonian $H_0 = \hbar\omega A^\dagger A$. The system is disturbed by the addition of a perturbing Hamiltonian $H_1 = g\hbar\omega(A + A^\dagger)$, where g is real. Show that the effect of the perturbation is to move the whole energy spectrum of the system down by $g^2\hbar\omega$.

19.8 For a system of N electrons in their ground state $|0\rangle$, the Hamiltonian is

$$H = \sum_{n=1}^{N} \frac{p_{x_n}^2 + p_{y_n}^2 + p_{z_n}^2}{2m} + \sum_{n=1}^{N} V(x_n, y_n, z_n).$$

Show that $\left[p_{x_n}^2, x_n\right] = -2i\hbar p_{x_n}$, and hence that the expectation value of the double commutator $[[x, H], x]$, where $x = \sum_{n=1}^{N} x_n$, is given by

$$\langle 0|\, [[x, H], x]\, |0\rangle = \frac{N\hbar^2}{m}.$$

Now evaluate the expectation value using the eigenvalue properties of H, namely $H|r\rangle = E_r|r\rangle$, and deduce the *sum rule for oscillation strengths*,

$$\sum_{r=0}^{\infty}(E_r - E_0)|\langle r\,|\,x\,|\,0\rangle\,|^2 = \frac{N\hbar^2}{2m}.$$

19.9 By considering the function

$$F(\lambda) = \exp(\lambda A)B\exp(-\lambda A),$$

where A and B are linear operators and λ is a parameter, and finding its derivatives with respect to λ, prove that

$$e^A Be^{-A} = B + [\,A, B\,] + \frac{1}{2!}\,[\,A, [\,A, B\,]\,] + \frac{1}{3!}\,[\,A, [\,A, [\,A, B\,]\,]\,] + \cdots.$$

Use this result to express

$$\exp\left(\frac{iL_x\theta}{\hbar}\right)\,L_y\,\exp\left(\frac{-iL_x\theta}{\hbar}\right)$$

as a linear combination of the angular momentum operators L_x, L_y and L_z.

19.10 For a system containing more than one particle, the total angular momentum J and its components are represented by operators that have completely analogous commutation relations to those for the operators for a single particle, i.e. J^2 has eigenvalue $j(j+1)\hbar^2$ and J_z has eigenvalue $m_j\hbar$ for the state $|j, m_j\rangle$. The usual orthonormality relationship $\langle j', m'_j\,|\,j, m_j\rangle = \delta_{j'j}\,\delta_{m'_j m_j}$ is also valid.

A system consists of two (distinguishable) particles A and B. Particle A is in an $\ell = 3$ state and can have state functions of the form $|A, 3, m_A\rangle$, whilst B is in an $\ell = 2$ state with possible state functions $|B, 2, m_B\rangle$. The range of possible values for j is $|3-2| \le j \le |3+2|$, i.e. $1 \le j \le 5$, and the overall state function can be written as

$$|j, m_j\rangle = \sum_{m_A+m_B=m_j} C^{j\,m_j}_{m_A\,m_B}\,|\,A, 3, m_A\rangle\,|\,B, 2, m_B\rangle.$$

The numerical coefficients $C^{j\,m_j}_{m_A\,m_B}$ are known as *Clebsch–Gordon* coefficients.

Assume (as can be shown) that the ladder operators $U(AB)$ and $D(AB)$ for the system can be written as $U(A) + U(B)$ and $D(A) + D(B)$, respectively, and that they lead to relationships equivalent to (19.34) and (19.35) with ℓ replaced by j and m by m_j.

(a) Apply the operators to the (obvious) relationship

$$|AB, 5, 5\rangle = |A, 3, 3\rangle\,|B, 2, 2\rangle$$

to show that

$$|AB, 5, 4\rangle = \sqrt{\tfrac{6}{10}}\,|A, 3, 2\rangle\,|B, 2, 2\rangle + \sqrt{\tfrac{4}{10}}\,|A, 3, 3\rangle\,|B, 2, 1\rangle.$$

(b) Find, to within an overall sign, the real coefficients c and d in the expansion

$$|AB, 4, 4\rangle = c|A, 3, 2\rangle\,|B, 2, 2\rangle + d|A, 3, 3\rangle\,|B, 2, 1\rangle$$

by requiring it to be orthogonal to $|AB, 5, 4\rangle$. Check your answer by considering $U(AB)|AB, 4, 4\rangle$.

(c) Find, to within an overall sign, and as efficiently as possible, an expression for $|AB, 4, -3\rangle$ as a sum of products of the form $|A, 3, m_A\rangle\,|B, 2, m_B\rangle$.

19.4 Hints and answers

19.1 Show that the commutator is anti-Hermitian.

19.3 Use the Hermitian conjugate of the given equation to obtain the time dependence of $\langle\psi|$. The rate of change of $\langle\psi|A|\psi\rangle$ is $i\langle\psi|\,[\,H, A\,]\,|\psi\rangle$. Note that $[\,H, p_x\,] = [\,V, p_x\,]$ and $[\,H, x\,] = \left[\,p_x^2, x\,\right]/2m$.

19.5 Show that $\mathsf{C}^2 = 2\mathsf{I}$.

$$\cos\mathsf{C} = \cos\sqrt{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sin\mathsf{C} = \frac{\sin\sqrt{2}}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

19.7 Express the total Hamiltonian in terms of $B = A + gI$ and determine the value of $\left[\,B, B^\dagger\,\right]$.

19.9 Show that, if $F^{(n)}$ is the nth derivative of $F(\lambda)$, then $F^{(n+1)} = \left[\,A, F^{(n)}\,\right]$. Use a Taylor series in λ to evaluate $F(1)$, using derivatives evaluated at $\lambda = 0$. Successively reduce the level of nesting of each multiple commutator by using the result of evaluating the previous term. The given expression reduces to $\cos\theta\, L_y - \sin\theta\, L_z$.

20

Partial differential equations: general and particular solutions

In this chapter and the next the solution of differential equations of types typically encountered in the physical sciences and engineering is extended to situations involving more than one independent variable. A partial differential equation (PDE) is an equation relating an unknown function (the dependent variable) of two or more variables to its partial derivatives with respect to those variables. The most commonly occurring independent variables are those describing position and time, and so we will couch our discussion and examples in notation appropriate to them.

As in other chapters we will focus our attention on the equations that arise most often in physical situations. We will restrict our discussion, therefore, to linear PDEs, i.e. those of first degree in the dependent variable. Furthermore, we will discuss primarily second-order equations. The solution of first-order PDEs will necessarily be involved in treating these, and some of the methods discussed can be extended without difficulty to third- and higher-order equations. We shall also see that many ideas developed for ordinary differential equations (ODEs) can be carried over directly into the study of PDEs.

In this chapter we will concentrate on general solutions of PDEs in terms of arbitrary functions and the particular solutions that may be derived from them in the presence of boundary conditions. We also discuss the existence and uniqueness of the solutions to PDEs under given boundary conditions.

In the next chapter the methods most commonly used in practice for obtaining solutions to PDEs subject to given boundary conditions will be considered. These methods include the separation of variables, integral transforms and Green's functions. This division of material is rather arbitrary and has been made only to emphasise the general usefulness of the latter methods. In particular, it will be readily apparent that some of the results of the present chapter are in fact solutions in the form of separated variables, but arrived at by a different approach.