22.3.1 Several dependent variables

Here we have $F = F(y_1, y_1', y_2, y_2', \ldots, y_n, y_n', x)$ where each $y_i = y_i(x)$. The analysis in this case proceeds as before, leading to n separate but simultaneous equations for the $y_i(x)$,

$$\frac{\partial F}{\partial y_i} = \frac{d}{dx}\left(\frac{\partial F}{\partial y_i'}\right), \qquad i = 1, 2, \ldots, n. \tag{22.12}$$

22.3.2 Several independent variables

With n independent variables, we need to extremise multiple integrals of the form

$$I = \int\int \cdots \int F\left(y, \frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \ldots, \frac{\partial y}{\partial x_n}, x_1, x_2, \ldots, x_n\right) dx_1\, dx_2 \cdots dx_n.$$

Using the same kind of analysis as before, we find that the extremising function $y = y(x_1, x_2, \ldots, x_n)$ must satisfy

$$\frac{\partial F}{\partial y} = \sum_{i=1}^{n} \frac{\partial}{\partial x_i}\left(\frac{\partial F}{\partial y_{x_i}}\right), \tag{22.13}$$

where y_{x_i} stands for $\partial y/\partial x_i$.

22.3.3 Higher-order derivatives

If in (22.1) $F = F(y, y', y'', \ldots, y^{(n)}, x)$ then using the same method as before and performing repeated integration by parts, it can be shown that the required extremising function $y(x)$ satisfies

$$\frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) + \frac{d^2}{dx^2}\left(\frac{\partial F}{\partial y''}\right) - \cdots + (-1)^n \frac{d^n}{dx^n}\left(\frac{\partial F}{\partial y^{(n)}}\right) = 0, \tag{22.14}$$

provided that $y = y' = \cdots = y^{(n-1)} = 0$ at both end-points. If y, or any of its derivatives, is not zero at the end-points then a corresponding contribution or contributions will appear on the RHS of (22.14).

22.3.4 Variable end-points

We now discuss the very important generalisation to variable end-points. Suppose, as before, we wish to find the function $y(x)$ that extremises the integral

$$I = \int_a^b F(y, y', x)\, dx,$$

but this time we demand only that the lower end-point is fixed, while we allow $y(b)$ to be arbitrary. Repeating the analysis of section 22.1, we find from (22.4)

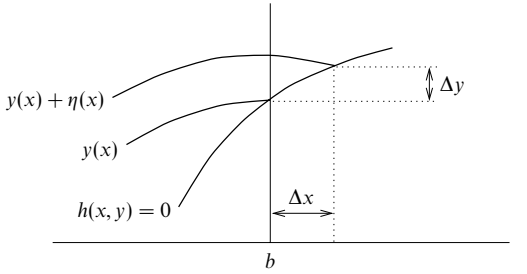


Figure 22.5 Variation of the end-point b along the curve $h(x, y) = 0$.

that we require

$$\left[\eta\frac{\partial F}{\partial y'}\right]_a^b + \int_a^b \left[\frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)\right]\eta(x)\,dx = 0. \tag{22.15}$$

Obviously the EL equation (22.5) must still hold for the second term on the LHS to vanish. Also, since the lower end-point is fixed, i.e. $\eta(a) = 0$, the first term on the LHS automatically vanishes at the lower limit. However, in order that it also vanishes at the upper limit, we require in addition that

$$\left.\frac{\partial F}{\partial y'}\right|_{x=b} = 0. \tag{22.16}$$

Clearly if both end-points may vary then $\partial F/\partial y'$ must vanish at both ends.

An interesting and more general case is where the lower end-point is again fixed at $x = a$, but the upper end-point is free to lie anywhere on the curve $h(x, y) = 0$. Now in this case, the variation in the value of I due to the arbitrary variation (22.2) is given to first order by

$$\delta I = \left[\frac{\partial F}{\partial y'}\eta\right]_a^b + \int_a^b \left(\frac{\partial F}{\partial y} - \frac{d}{dx}\frac{\partial F}{\partial y'}\right)\eta\,dx + F(b)\Delta x, \tag{22.17}$$

where Δx is the displacement in the x-direction of the upper end-point, as indicated in figure 22.5, and $F(b)$ is the value of F at $x = b$. In order for (22.17) to be valid, we of course require the displacement Δx to be small.

From the figure we see that $\Delta y = \eta(b) + y'(b)\Delta x$. Since the upper end-point must lie on $h(x, y) = 0$ we also require that, at $x = b$,

$$\frac{\partial h}{\partial x}\Delta x + \frac{\partial h}{\partial y}\Delta y = 0,$$

which on substituting our expression for Δy and rearranging becomes

$$\left(\frac{\partial h}{\partial x} + y'\frac{\partial h}{\partial y}\right)\Delta x + \frac{\partial h}{\partial y}\eta = 0. \tag{22.18}$$

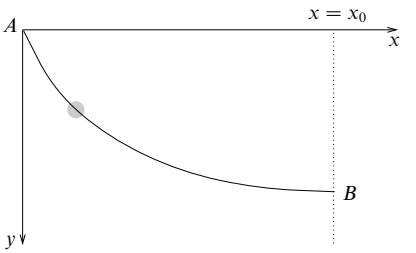


Figure 22.6 A frictionless wire along which a small bead slides. We seek the shape of the wire that allows the bead to travel from the origin O to the line $x = x_0$ in the least possible time.

Now, from (22.17) the condition $\delta I = 0$ requires, besides the EL equation, that at $x = b$, the other two contributions cancel, i.e.

$$F\Delta x + \frac{\partial F}{\partial y'}\eta = 0. \tag{22.19}$$

Eliminating Δx and η between (22.18) and (22.19) leads to the condition that at the end-point

$$\left(F - y'\frac{\partial F}{\partial y'}\right)\frac{\partial h}{\partial y} - \frac{\partial F}{\partial y'}\frac{\partial h}{\partial x} = 0. \tag{22.20}$$

In the special case where the end-point is free to lie anywhere on the vertical line $x = b$, we have $\partial h/\partial x = 1$ and $\partial h/\partial y = 0$. Substituting these values into (22.20), we recover the end-point condition given in (22.16).

►*A frictionless wire in a vertical plane connects two points A and B, A being higher than B. Let the position of A be fixed at the origin of an xy-coordinate system, but allow B to lie anywhere on the vertical line $x = x_0$ (see figure 22.6). Find the shape of the wire such that a bead placed on it at A will slide under gravity to B in the shortest possible time.*

This is a variant of the famous brachistochrone (shortest time) problem, which is often used to illustrate the calculus of variations. Conservation of energy tells us that the particle speed is given by

$$v = \frac{ds}{dt} = \sqrt{2gy},$$

where s is the path length along the wire and g is the acceleration due to gravity. Since the element of path length is $ds = (1 + y'^2)^{1/2}dx$, the total time taken to travel to the line $x = x_0$ is given by

$$t = \int_{x=0}^{x=x_0} \frac{ds}{v} = \frac{1}{\sqrt{2g}}\int_0^{x_0} \sqrt{\frac{1+y'^2}{y}}\,dx.$$

Because the integrand does not contain x explicitly, we can use (22.8) with the specific form $F = \sqrt{1+y'^2}/\sqrt{y}$ to find a first integral; on simplification this yields

$$\left[y(1+y'^2)\right]^{1/2} = k,$$

where k is a constant. Letting $a = k^2$ and solving for y' we find

$$y' = \frac{dy}{dx} = \sqrt{\frac{a-y}{y}},$$

which on substituting $y = a\sin^2\theta$ integrates to give

$$x = \frac{a}{2}(2\theta - \sin 2\theta) + c.$$

Thus the parametric equations of the curve are given by

$$x = b(\phi - \sin\phi) + c, \qquad y = b(1 - \cos\phi),$$

where $b = a/2$ and $\phi = 2\theta$; they define a cycloid, the curve traced out by a point on the rim of a wheel of radius b rolling along the x-axis. We must now use the end-point conditions to determine the constants b and c. Since the curve passes through the origin, we see immediately that $c = 0$. Now since $y(x_0)$ is arbitrary, i.e. the upper end-point can lie anywhere on the curve $x = x_0$, the condition (22.20) reduces to (22.16), so that we also require

$$\left.\frac{\partial F}{\partial y'}\right|_{x=x_0} = \left.\frac{y'}{\sqrt{y(1+y'^2)}}\right|_{x=x_0} = 0,$$

which implies that $y' = 0$ at $x = x_0$. In words, the tangent to the cycloid at B must be parallel to the x-axis; this requires $\pi b = x_0$. ◄

22.4 Constrained variation

Just as the problem of finding thestationary values of a function $f(x, y)$ subject to the constraint $g(x, y) =$ constant is solved by means of Lagrange's undetermined multipliers (see chapter 5), so the corresponding problem in the calculus of variations is solved by an analogous method.

Suppose that we wish to find the stationary values of

$$I = \int_a^b F(y, y', x)\,dx,$$

subject to the constraint that the value of

$$J = \int_a^b G(y, y', x)\,dx$$

is held constant. Following the method of Lagrange undetermined multipliers let us define a new functional

$$K = I + \lambda J = \int_a^b (F + \lambda G)\,dx,$$

and find its *unconstrained* stationary values. Repeating the analysis of section 22.1 we find that we require

$$\frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) + \lambda\left[\frac{\partial G}{\partial y} - \frac{d}{dx}\left(\frac{\partial G}{\partial y'}\right)\right] = 0,$$

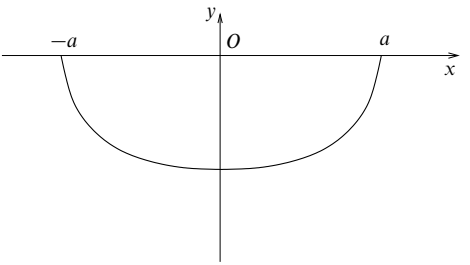


Figure 22.7 A uniform rope with fixed end-points suspended under gravity.

which, together with the original constraint $J =$ constant, will yield the required solution $y(x)$.

This method is easily generalised to cases with more than one constraint by the introduction of more Lagrange multipliers. If we wish to find the stationary values of an integral I subject to the multiple constraints that the values of the integrals J_i be held constant for $i = 1, 2, \ldots, n$, then we simply find the unconstrained stationary values of the new integral

$$K = I + \sum_{1}^{n} \lambda_i J_i.$$

►*Find the shape assumed by a uniform rope when suspended by its ends from two points at equal heights.*

We will solve this problem using x (see figure 22.7) as the independent variable. Let the rope of length $2L$ be suspended between the points $x = \pm a$, $y = 0$ ($L > a$) and have uniform linear density ρ. We then need to find the stationary value of the rope's gravitational potential energy,

$$I = -\rho g \int y \, ds = -\rho g \int_{-a}^{a} y(1 + y'^2)^{1/2} \, dx,$$

with respect to small changes in the form of the rope but subject to the constraint that the total length of the rope remains constant, i.e.

$$J = \int ds = \int_{-a}^{a} (1 + y'^2)^{1/2} \, dx = 2L.$$

We thus define a new integral (omitting the factor -1 from I for brevity)

$$K = I + \lambda J = \int_{-a}^{a} (\rho g y + \lambda)(1 + y'^2)^{1/2} \, dx$$

and find its stationary values. Since the integrand does not contain the independent variable x explicitly, we can use (22.8) to find the first integral:

$$(\rho g y + \lambda)\left(1 + y'^2\right)^{1/2} - (\rho g y + \lambda)\left(1 + y'^2\right)^{-1/2} y'^2 = k,$$

where k is a constant; this reduces to

$$y'^2 = \left(\frac{\rho g y + \lambda}{k}\right)^2 - 1.$$

Making the substitution $\rho g y + \lambda = k \cosh z$, this can be integrated easily to give

$$\frac{k}{\rho g} \cosh^{-1}\left(\frac{\rho g y + \lambda}{k}\right) = x + c,$$

where c is the constant of integration.

We now have three unknowns, λ, k and c, that must be evaluated using the two end conditions $y(\pm a) = 0$ and the constraint $J = 2L$. The end conditions give

$$\cosh\frac{\rho g(a+c)}{k} = \frac{\lambda}{k} = \cosh\frac{\rho g(-a+c)}{k},$$

and since $a \neq 0$, these imply $c = 0$ and $\lambda/k = \cosh(\rho g a/k)$. Putting $c = 0$ into the constraint, in which $y' = \sinh(\rho g x/k)$, we obtain

$$\begin{aligned} 2L &= \int_{-a}^{a} \left[1 + \sinh^2\left(\frac{\rho g x}{k}\right)\right]^{1/2} dx \\ &= \frac{2k}{\rho g} \sinh\left(\frac{\rho g a}{k}\right). \end{aligned}$$

Collecting together the values for the constants, the form adopted by the rope is therefore

$$y(x) = \frac{k}{\rho g}\left[\cosh\left(\frac{\rho g x}{k}\right) - \cosh\left(\frac{\rho g a}{k}\right)\right],$$

where k is the solution of $\sinh(\rho g a/k) = \rho g L/k$. This curve is known as a catenary. ◄

22.5 Physical variational principles

Many results in both classical and quantum physics can be expressed as variational principles, and it is often when expressed in this form that their physical meaning is most clearly understood. Moreover, once a physical phenomenon has been written as a variational principle, we can use all the results derived in this chapter to investigate its behaviour. It is usually possible to identify conserved quantities, or symmetries of the system of interest, that otherwise might be found only with considerable effort. From the wide range of physical variational principles we will select two examples from familiar areas of classical physics, namely geometric optics and mechanics.

22.5.1 Fermat's principle in optics

Fermat's principle in geometrical optics states that a ray of light travelling in a region of variable refractive index follows a path such that the total optical path length (physical length × refractive index) is stationary.

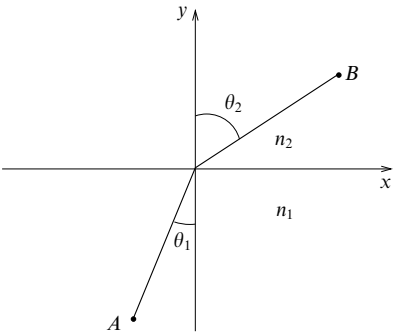


Figure 22.8 Path of a light ray at the plane interface between media with refractive indices n_1 and n_2, where $n_2 < n_1$.

►*From Fermat's principle deduce Snell's law of refraction at an interface.*

Let the interface be at $y =$ constant (see figure 22.8) and let it separate two regions with refractive indices n_1 and n_2 respectively. On a ray the element of physical path length is $ds = (1 + y'^2)^{1/2}dx$, and so for a ray that passes through the points A and B, the total optical path length is

$$P = \int_A^B n(y)(1 + y'^2)^{1/2}\,dx.$$

Since the integrand does not contain the independent variable x explicitly, we use (22.8) to obtain a first integral, which, after some rearrangement, reads

$$n(y)\left(1 + y'^2\right)^{-1/2} = k,$$

where k is a constant. Recalling that y' is the tangent of the angle ϕ between the instantaneous direction of the ray and the x-axis, this *general* result, which is not dependent on the configuration presently under consideration, can be put in the form

$$n\cos\phi = \text{ constant}$$

along a ray, even though n and ϕ vary individually.

For our particular configuration n is constant in each medium and therefore so is y'. Thus the rays travel in straight lines in each medium (as anticipated in figure 22.8, but not assumed in our analysis), and since k is constant along the *whole* path we have $n_1\cos\phi_1 = n_2\cos\phi_2$, or in terms of the conventional angles in the figure

$$n_1\sin\theta_1 = n_2\sin\theta_2.\ \blacktriangleleft$$

22.5.2 Hamilton's principle in mechanics

Consider a mechanical system whose configuration can be uniquely defined by a number of coordinates q_i (usually distances and angles) together with time t and which experiences only forces derivable from a potential. Hamilton's principle

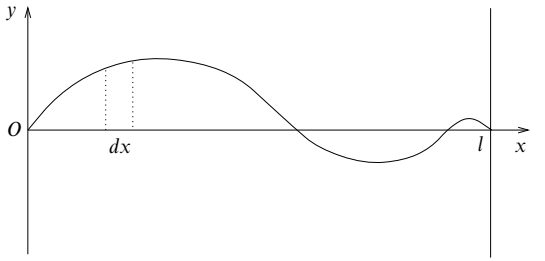


Figure 22.9 Transverse displacement on a taut string that is fixed at two points a distance l apart.

states that in moving from one configuration at time t_0 to another at time t_1 the motion of such a system is such as to make

$$\mathcal{L} = \int_{t_0}^{t_1} L(q_1, q_2 \ldots, q_n, \dot{q}_1, \dot{q}_2, \ldots, \dot{q}_n, t)\, dt \tag{22.21}$$

stationary. The *Lagrangian* L is defined, in terms of the kinetic energy T and the potential energy V (with respect to some reference situation), by $L = T - V$. Here V is a function of the q_i only, not of the $\dot{q}_i$. Applying the EL equation to $\mathcal{L}$ we obtain *Lagrange's equations*,

$$\frac{\partial L}{\partial q_i} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right), \qquad i = 1, 2, \ldots, n.$$

►*Using Hamilton's principle derive the wave equation for small transverse oscillations of a taut string.*

In this example we are in fact considering a generalisation of (22.21) to a case involving one isolated independent coordinate t, together with a *continuum* in which the q_i become the continuous variable x. The expressions for T and V therefore become integrals over x rather than sums over the label i.

If ρ and τ are the local density and tension of the string, both of which may depend on x, then, referring to figure 22.9, the kinetic and potential energies of the string are given by

$$T = \int_0^l \frac{\rho}{2}\left(\frac{\partial y}{\partial t}\right)^2 dx, \qquad V = \int_0^l \frac{\tau}{2}\left(\frac{\partial y}{\partial x}\right)^2 dx$$

and (22.21) becomes

$$\mathcal{L} = \frac{1}{2}\int_{t_0}^{t_1} dt \int_0^l \left[\rho\left(\frac{\partial y}{\partial t}\right)^2 - \tau\left(\frac{\partial y}{\partial x}\right)^2\right] dx.$$

Using (22.13) and the fact that y does not appear explicitly, we obtain

$$\frac{\partial}{\partial t}\left(\rho\frac{\partial y}{\partial t}\right) - \frac{\partial}{\partial x}\left(\tau\frac{\partial y}{\partial x}\right) = 0.$$

If, in addition, ρ and τ do not depend on x or t then

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 y}{\partial t^2},$$

where $c^2 = \tau/\rho$. This is the wave equation for small transverse oscillations of a taut uniform string. ◄

22.6 General eigenvalue problems

We have seen in this chapter that the problem of finding a curve that makes the value of a given integral stationary when the integral is taken along the curve results, in each case, in a differential equation for the curve. It is not a great extension to ask whether this may be used to solve differential equations, by setting up a suitable variational problem and then seeking ways other than the Euler equation of finding or estimating stationary solutions.

We shall be concerned with differential equations of the form $\mathcal{L}y = \lambda\rho(x)y$, where the differential operator $\mathcal{L}$ is self-adjoint, so that $\mathcal{L} = \mathcal{L}^\dagger$ (with appropriate boundary conditions on the solution y) and $\rho(x)$ is some weight function, as discussed in chapter 17. In particular, we will concentrate on the Sturm–Liouville equation as an explicit example, but much of what follows can be applied to other equations of this type.

We have already discussed the solution of equations of the Sturm–Liouville type in chapter 17 and the same notation will be used here. In this section, however, we will adopt a variational approach to estimating the eigenvalues of such equations.

Suppose we search for stationary values of the integral

$$I = \int_a^b \left[p(x)y'^2(x) - q(x)y^2(x)\right]\,dx, \tag{22.22}$$

with $y(a) = y(b) = 0$ and p and q any sufficiently smooth and differentiable functions of x. However, in addition we impose a normalisation condition

$$J = \int_a^b \rho(x)y^2(x)\,dx = \text{constant}. \tag{22.23}$$

Here $\rho(x)$ is a positive weight function defined in the interval $a \le x \le b$, but which may in particular cases be a constant.

Then, as in section 22.4, we use undetermined Lagrange multipliers,[§] and

[§] We use $-\lambda$, rather than λ, so that the final equation (22.24) appears in the conventional Sturm–Liouville form.

consider $K = I - \lambda J$ given by

$$K = \int_a^b \left[py'^2 - (q + \lambda\rho)y^2 \right] dx.$$

On application of the EL equation (22.5) this yields

$$\frac{d}{dx}\left(p\frac{dy}{dx}\right) + qy + \lambda\rho y = 0, \tag{22.24}$$

which is exactly the Sturm–Liouville equation (17.34), with eigenvalue λ. Now, since both I and J are quadratic in y and its derivative, finding stationary values of K is equivalent to finding stationary values of I/J. This may also be shown by considering the functional $\Lambda = I/J$, for which

$$\begin{aligned}\delta\Lambda &= (\delta I/J) - (I/J^2)\,\delta J \\ &= (\delta I - \Lambda\delta J)/J \\ &= \delta K/J.\end{aligned}$$

Hence, extremising Λ is equivalent to extremising K. Thus we have the important result that *finding functions y that make I/J stationary is equivalent to finding functions y that are solutions of the Sturm–Liouville equation; the resulting value of I/J equals the corresponding eigenvalue of the equation.*

Of course this does not tell us how to find such a function y and, naturally, to have to do this by solving (22.24) directly defeats the purpose of the exercise. We will see in the next section how some progress can be made. It is worth recalling that the functions $p(x)$, $q(x)$ and $\rho(x)$ can have many different forms, and so (22.24) represents quite a wide variety of equations.

We now recall some properties of the solutions of the Sturm–Liouville equation. The eigenvalues λ_i of (22.24) are real and will be assumed non-degenerate (for simplicity). We also assume that the corresponding eigenfunctions have been made real, so that normalised eigenfunctions $y_i(x)$ satisfy the orthogonality relation (as in (17.24))

$$\int_a^b y_i y_j \rho\, dx = \delta_{ij}. \tag{22.25}$$

Further, we take the boundary condition in the form

$$\left[y_i p y_j' \right]_{x=a}^{x=b} = 0; \tag{22.26}$$

this can be satisfied by $y(a) = y(b) = 0$, but also by many other sets of boundary conditions.

►*Show that*

$$\int_a^b \left(y_j' p y_i' - y_j q y_i\right)\, dx = \lambda_i \delta_{ij}. \tag{22.27}$$

Let y_i be an eigenfunction of (22.24), corresponding to a particular eigenvalue λ_i, so that

$$\left(py_i'\right)' + (q + \lambda_i \rho) y_i = 0.$$

Multiplying this through by y_j and integrating from a to b (the first term by parts) we obtain

$$\left[y_j \left(py_i'\right)\right]_a^b - \int_a^b y_j'(py_i')\, dx + \int_a^b y_j(q + \lambda_i \rho) y_i\, dx = 0. \tag{22.28}$$

The first term vanishes by virtue of (22.26), and on rearranging the other terms and using (22.25), we find the result (22.27). ◄

We see at once that, if the function $y(x)$ minimises I/J, i.e. satisfies the Sturm–Liouville equation, then putting $y_i = y_j = y$ in (22.25) and (22.27) yields J and I respectively on the left-hand sides; thus, as mentioned above, the minimised value of I/J is just the eigenvalue λ, introduced originally as the undetermined multiplier.

►*For a function y satisfying the Sturm–Liouville equation verify that, provided (22.26) is satisfied, $\lambda = I/J$.*

Firstly, we multiply (22.24) through by y to give

$$y(py')' + qy^2 + \lambda \rho y^2 = 0.$$

Now integrating this expression by parts we have

$$\left[ypy'\right]_a^b - \int_a^b \left(py'^2 - qy^2\right)\, dx + \lambda \int_a^b \rho y^2\, dx = 0.$$

The first term on the LHS is zero, the second is simply $-I$ and the third is λJ. Thus $\lambda = I/J$. ◄

22.7 Estimation of eigenvalues and eigenfunctions

Since the eigenvalues λ_i of the Sturm–Liouville equation are the stationary values of I/J (see above), it follows that any evaluation of I/J must yield a value that lies between the lowest and highest eigenvalues of the corresponding Sturm–Liouville equation, i.e.

$$\lambda_{\min} \leq \frac{I}{J} \leq \lambda_{\max},$$

where, depending on the equation under consideration, either $\lambda_{\min} = -\infty$ and

$\lambda_{\max}$ is finite, or $\lambda_{\max} = \infty$ and $\lambda_{\min}$ is finite. Notice that here we have departed from direct consideration of the minimising problem and made a statement about a calculation in which no actual minimisation is necessary.

Thus, as an example, for an equation with a finite lowest eigenvalue λ_0 any evaluation of I/J provides an upper bound on λ_0. Further, we will now show that the estimate λ obtained is a better estimate of λ_0 than the estimated (guessed) function y is of y_0, the true eigenfunction corresponding to λ_0. The sense in which 'better' is used here will be clear from the final result.

Firstly, we expand the estimated or *trial function* y in terms of the complete set y_i:

$$y = y_0 + c_1 y_1 + c_2 y_2 + \cdots,$$

where, if a good trial function has been guessed, the c_i will be small. Using (22.25) we have immediately that $J = 1 + \sum_i |c_i|^2$. The other required integral is

$$I = \int_a^b \left[p\left(y_0' + \sum_i c_i y_i' \right)^2 - q\left(y_0 + \sum_i c_i y_i \right)^2 \right] dx.$$

On multiplying out the squared terms, all the cross terms vanish because of (22.27) to leave

$$\begin{aligned} \lambda &= \frac{I}{J} \\ &= \frac{\lambda_0 + \sum_i |c_i|^2 \lambda_i}{1 + \sum_j |c_j|^2} \\ &= \lambda_0 + \sum_i |c_i|^2 (\lambda_i - \lambda_0) + \mathrm{O}(c^4). \end{aligned}$$

Hence λ differs from λ_0 by a term second order in the c_i, even though y differed from y_0 by a term first order in the c_i; this is what we aimed to show. We notice incidentally that, since $\lambda_0 < \lambda_i$ for all i, λ is shown to be necessarily $\geq \lambda_0$, with equality only if all $c_i = 0$, i.e. if $y \equiv y_0$.

The method can be extended to the second and higher eigenvalues by imposing, in addition to the original constraints and boundary conditions, a restriction of the trial functions to only those that are orthogonal to the eigenfunctions corresponding to lower eigenvalues. (Of course, this requires complete or nearly complete knowledge of these latter eigenfunctions.) An example is given at the end of the chapter (exercise 22.25).

We now illustrate the method we have discussed by considering a simple example, one for which, as on previous occasions, the answer is obvious.

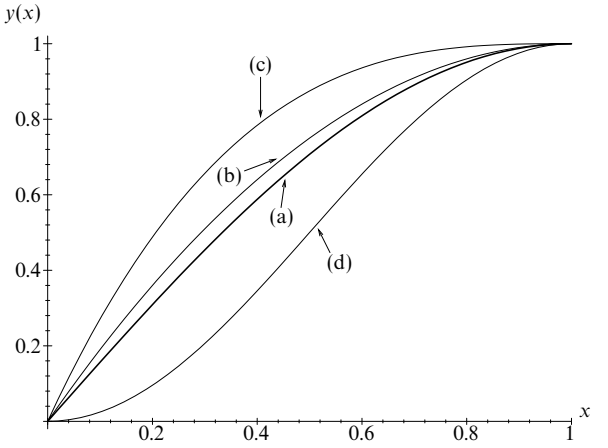


Figure 22.10 Trial solutions used to estimate the lowest eigenvalue λ of $-y'' = \lambda y$ with $y(0) = y'(1) = 0$. They are: (a) $y = \sin(\pi x/2)$, the exact result; (b) $y = 2x - x^2$; (c) $y = x^3 - 3x^2 + 3x$; (d) $y = \sin^2(\pi x/2)$.

► *Estimate the lowest eigenvalue of the equation*

$$-\frac{d^2y}{dx^2} = \lambda y, \qquad 0 \le x \le 1, \tag{22.29}$$

with boundary conditions

$$y(0) = 0, \qquad y'(1) = 0. \tag{22.30}$$

We need to find the lowest value λ_0 of λ for which (22.29) has a solution $y(x)$ that satisfies (22.30). The exact answer is of course $y = A\sin(x\pi/2)$ and $\lambda_0 = \pi^2/4 \approx 2.47$.

Firstly we note that the Sturm–Liouville equation reduces to (22.29) if we take $p(x) = 1$, $q(x) = 0$ and $\rho(x) = 1$ and that the boundary conditions satisfy (22.26). Thus we are able to apply the previous theory.

We will use three trial functions so that the effect on the estimate of λ_0 of making better or worse 'guesses' can be seen. One further preliminary remark is relevant, namely that the estimate is independent of any constant multiplicative factor in the function used. This is easily verified by looking at the form of I/J. We normalise each trial function so that $y(1) = 1$, purely in order to facilitate comparison of the various function shapes.

Figure 22.10 illustrates the trial functions used, curve (a) being the exact solution $y = \sin(\pi x/2)$. The other curves are (b) $y(x) = 2x - x^2$, (c) $y(x) = x^3 - 3x^2 + 3x$, and (d) $y(x) = \sin^2(\pi x/2)$. The choice of trial function is governed by the following considerations:

(i) the boundary conditions (22.30) *must* be satisfied.
(ii) a 'good' trial function ought to mimic the correct solution as far as possible, but it may not be easy to guess even the general shape of the correct solution in some cases.
(iii) the evaluation of I/J should be as simple as possible.

It is easily verified that functions (b), (c) and (d) all satisfy (22.30) but, so far as mimicking the correct solution is concerned, we would expect from the figure that (b) would be superior to the other two. The three evaluations are straightforward, using (22.22) and (22.23):

$$\lambda_b = \frac{\int_0^1 (2-2x)^2\,dx}{\int_0^1 (2x-x^2)^2\,dx} = \frac{4/3}{8/15} = 2.50$$

$$\lambda_c = \frac{\int_0^1 (3x^2-6x+3)^2\,dx}{\int_0^1 (x^3-3x^2+3x)^2\,dx} = \frac{9/5}{9/14} = 2.80$$

$$\lambda_d = \frac{\int_0^1 (\pi^2/4)\sin^2(\pi x)\,dx}{\int_0^1 \sin^4(\pi x/2)\,dx} = \frac{\pi^2/8}{3/8} = 3.29.$$

We expected all evaluations to yield estimates greater than the lowest eigenvalue, 2.47, and this is indeed so. From these trials alone we are able to say (only) that $\lambda_0 \leq 2.50$. As expected, the best approximation (b) to the true eigenfunction yields the lowest, and therefore the best, upper bound on λ_0. ◀

We may generalise the work of this section to other differential equations of the form $\mathcal{L}y = \lambda\rho y$, where $\mathcal{L} = \mathcal{L}^\dagger$. In particular, one finds

$$\lambda_{\min} \leq \frac{I}{J} \leq \lambda_{\max},$$

where I and J are now given by

$$I = \int_a^b y^*(\mathcal{L}y)\,dx \qquad \text{and} \qquad J = \int_a^b \rho y^* y\,dx. \tag{22.31}$$

It is straightforward to show that, for the special case of the Sturm–Liouville equation, for which

$$\mathcal{L}y = -(py')' - qy,$$

the expression for I in (22.31) leads to (22.22).

22.8 Adjustment of parameters

Instead of trying to estimate λ_0 by selecting a large number of different trial functions, we may also use trial functions that include one or more parameters which themselves may be adjusted to give the lowest value to $\lambda = I/J$ and hence the best estimate of λ_0. The justification for this method comes from the knowledge that no matter what form of function is chosen, nor what values are assigned to the parameters, provided the boundary conditions are satisfied λ can never be less than the required λ_0.

To illustrate this method an example from quantum mechanics will be used. The time-independent Schrödinger equation is formally written as the eigenvalue equation $H\psi = E\psi$, where H is a linear operator, ψ the wavefunction describing a quantum mechanical system and E the energy of the system. The energy

operator H is called the Hamiltonian and for a particle of mass m moving in a one-dimensional harmonic oscillator potential is given by

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{kx^2}{2}, \tag{22.32}$$

where $\hbar$ is Planck's constant divided by 2π.

►*Estimate the ground-state energy of a quantum harmonic oscillator.*

Using (22.32) in $H\psi = E\psi$, the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{kx^2}{2}\psi = E\psi, \qquad -\infty < x < \infty. \tag{22.33}$$

The boundary conditions are that ψ should vanish as $x \to \pm\infty$. Equation (22.33) is a form of the Sturm–Liouville equation in which $p = \hbar^2/(2m)$, $q = -kx^2/2$, $\rho = 1$ and $\lambda = E$; it can be solved by the methods developed previously, e.g. by writing the eigenfunction ψ as a power series in x.

However, our purpose here is to illustrate variational methods and so we take as a trial wavefunction $\psi = \exp(-\alpha x^2)$, where α is a positive parameter whose value we will choose later. This function certainly $\to 0$ as $x \to \pm\infty$ and is convenient for calculations. Whether it approximates the true wave function is unknown, but if it does not our estimate will still be valid, although the upper bound will be a poor one.

With $y = \exp(-\alpha x^2)$ and therefore $y' = -2\alpha x \exp(-\alpha x^2)$, the required estimate is

$$E = \lambda = \frac{\int_{-\infty}^{\infty}[(\hbar^2/2m)4\alpha^2x^2 + (k/2)x^2]e^{-2\alpha x^2}\,dx}{\int_{-\infty}^{\infty} e^{-2\alpha x^2}\,dx} = \frac{\hbar^2\alpha}{2m} + \frac{k}{8\alpha}. \tag{22.34}$$

This evaluation is easily carried out using the reduction formula

$$I_n = \frac{n-1}{4\alpha}I_{n-2}, \quad \text{for integrals of the form} \quad I_n = \int_{-\infty}^{\infty} x^n e^{-2\alpha x^2}\,dx. \tag{22.35}$$

So, we have obtained the estimate (22.34), involving the parameter α, for the oscillator's ground-state energy, i.e. the lowest eigenvalue of H. In line with our previous discussion we now minimise λ with respect to α. Putting $d\lambda/d\alpha = 0$ (clearly a minimum), yields $\alpha = (km)^{1/2}/(2\hbar)$, which in turn gives as the minimum value for λ

$$E = \frac{\hbar}{2}\left(\frac{k}{m}\right)^{1/2} = \frac{\hbar\omega}{2}, \tag{22.36}$$

where we have put $(k/m)^{1/2}$ equal to the classical angular frequency ω.

The method thus leads to the conclusion that the ground-state energy E_0 is $\leq \frac{1}{2}\hbar\omega$. In fact, as is well known, the equality sign holds, $\frac{1}{2}\hbar\omega$ being just the zero-point energy of a quantum mechanical oscillator. Our estimate gives the exact value because $\psi(x) = \exp(-\alpha x^2)$ is the correct functional form for the ground state wavefunction and the particular value of α that we have found is that needed to make ψ an eigenfunction of H with eigenvalue $\frac{1}{2}\hbar\omega$. ◄

An alternative but equivalent approach to this is developed in the exercises that follow, as is an extension of this particular problem to estimating the second-lowest eigenvalue (see exercise 22.25).

22.9 Exercises

22.1 A surface of revolution, whose equation in cylindrical polar coordinates is $\rho = \rho(z)$, is bounded by the circles $\rho = a$, $z = \pm c$ $(a > c)$. Show that the function that makes the surface integral $I = \int \rho^{-1/2}\, dS$ stationary with respect to small variations is given by $\rho(z) = k + z^2/(4k)$, where $k = [a \pm (a^2 - c^2)^{1/2}]/2$.

22.2 Show that the lowest value of the integral

$$\int_A^B \frac{(1 + y'^2)^{1/2}}{y}\, dx,$$

where A is $(-1, 1)$ and B is $(1, 1)$, is $2\ln(1+\sqrt{2})$. Assume that the Euler–Lagrange equation gives a minimising curve.

22.3 The refractive index n of a medium is a function only of the distance r from a fixed point O. Prove that the equation of a light ray, assumed to lie in a plane through O, travelling in the medium satisfies (in plane polar coordinates)

$$\frac{1}{r^2}\left(\frac{dr}{d\phi}\right)^2 = \frac{r^2}{a^2}\frac{n^2(r)}{n^2(a)} - 1,$$

where a is the distance of the ray from O at the point at which $dr/d\phi = 0$.

If $n = [1 + (\alpha^2/r^2)]^{1/2}$ and the ray starts and ends far from O, find its deviation (the angle through which the ray is turned), if its minimum distance from O is a.

22.4 The Lagrangian for a π-meson is given by

$$L(\mathbf{x}, t) = \tfrac{1}{2}(\dot{\phi}^2 - |\nabla\phi|^2 - \mu^2\phi^2),$$

where μ is the meson mass and $\phi(\mathbf{x}, t)$ is its wavefunction. Assuming Hamilton's principle, find the wave equation satisfied by ϕ.

22.5 Prove the following results about general systems.

(a) For a system described in terms of coordinates q_i and t, show that if t does not appear explicitly in the expressions for x, y and z ($x = x(q_i, t)$, etc.) then the kinetic energy T is a homogeneous quadratic function of the $\dot{q}_i$ (it may also involve the q_i). Deduce that $\sum_i \dot{q}_i(\partial T/\partial \dot{q}_i) = 2T$.

(b) Assuming that the forces acting on the system are derivable from a potential V, show, by expressing dT/dt in terms of q_i and $\dot{q}_i$, that $d(T + V)/dt = 0$.

22.6 For a system specified by the coordinates q and t, show that the equation of motion is unchanged if the Lagrangian $L(q, \dot{q}, t)$ is replaced by

$$L_1 = L + \frac{d\phi(q, t)}{dt},$$

where ϕ is an arbitrary function. Deduce that the equation of motion of a particle that moves in one dimension subject to a force $-dV(x)/dx$ (x being measured from a point O) is unchanged if O is forced to move with a constant velocity v (x still being measured from O).

22.7 In cylindrical polar coordinates, the curve $(\rho(\theta), \theta, \alpha\rho(\theta))$ lies on the surface of the cone $z = \alpha\rho$. Show that geodesics (curves of minimum length joining two points) on the cone satisfy

$$\rho^4 = c^2[\beta^2\rho'^2 + \rho^2],$$

where c is an arbitrary constant, but β has to have a particular value. Determine the form of $\rho(\theta)$ and hence find the equation of the shortest path on the cone between the points $(R, -\theta_0, \alpha R)$ and $(R, \theta_0, \alpha R)$.

[You will find it useful to determine the form of the derivative of $\cos^{-1}(u^{-1})$.]

22.8 Derive the differential equations for the plane-polar coordinates, r and ϕ, of a particle of unit mass moving in a field of potential $V(r)$. Find the form of V if the path of the particle is given by $r = a\sin\phi$.

22.9 You are provided with a line of length $\pi a/2$ and negligible mass and some lead shot of total mass M. Use a variational method to determine how the lead shot must be distributed along the line if the loaded line is to hang in a circular arc of radius a when its ends are attached to two points at the same height. Measure the distance s along the line from its centre.

22.10 Extend the result of subsection 22.2.2 to the case of several dependent variables $y_i(x)$, showing that, if x does not appear explicitly in the integrand, then a first integral of the Euler–Lagrange equations is

$$F - \sum_{i=1}^{n} y_i' \frac{\partial F}{\partial y_i'} = \text{constant}.$$

22.11 A general result is that light travels through a variable medium by a path which minimises the travel time (this is an alternative formulation of Fermat's principle). With respect to a particular cylindrical polar coordinate system (ρ, ϕ, z), the speed of light $v(\rho, \phi)$ is independent of z. If the path of the light is parameterised as $\rho = \rho(z), \phi = \phi(z)$, use the result of the previous exercise to show that

$$v^2(\rho'^2 + \rho^2\phi'^2 + 1)$$

is constant along the path.

For the particular case when $v = v(\rho) = b(a^2 + \rho^2)^{1/2}$, show that the two Euler–Lagrange equations have a common solution in which the light travels along a helical path given by $\phi = Az + B$, $\rho = C$, provided that A has a particular value.

22.12 Light travels in the vertical xz-plane through a slab of material which lies between the planes $z = z_0$ and $z = 2z_0$, and in which the speed of light $v(z) = c_0 z/z_0$. Using the alternative formulation of Fermat's principle, given in the previous question, show that the ray paths are arcs of circles.

Deduce that, if a ray enters the material at $(0, z_0)$ at an angle to the vertical, $\pi/2 - \theta$, of more than 30°, then it does not reach the far side of the slab.

22.13 A dam of capacity V (less than $\pi b^2 h/2$) is to be constructed on level ground next to a long straight wall which runs from $(-b, 0)$ to $(b, 0)$. This is to be achieved by joining the ends of a new wall, of height h, to those of the existing wall. Show that, in order to minimise the length L of new wall to be built, it should form part of a circle, and that L is then given by

$$\int_{-b}^{b} \frac{dx}{(1 - \lambda^2 x^2)^{1/2}},$$

where λ is found from

$$\frac{V}{hb^2} = \frac{\sin^{-1}\mu}{\mu^2} - \frac{(1 - \mu^2)^{1/2}}{\mu}$$

and $\mu = \lambda b$.

22.14 In the brachistochrone problem of subsection 22.3.4 show that if the upper end-point can lie anywhere on the curve $h(x, y) = 0$, then the curve of quickest descent $y(x)$ meets $h(x, y) = 0$ at right angles.

22.15 The Schwarzchild metric for the static field of a non-rotating spherically symmetric black hole of mass M is given by

$$(ds)^2 = c^2\left(1 - \frac{2GM}{c^2 r}\right)(dt)^2 - \frac{(dr)^2}{1 - 2GM/(c^2 r)} - r^2(d\theta)^2 - r^2\sin^2\theta\,(d\phi)^2.$$

Considering only motion confined to the plane $\theta = \pi/2$, and assuming that the

path of a small test particle is such as to make $\int ds$ stationary, find two first integrals of the equations of motion. From their Newtonian limits, in which GM/r, $\dot{r}^2$ and $r^2\dot{\phi}^2$ are all $\ll c^2$, identify the constants of integration.

22.16 Use result (22.27) to evaluate

$$J = \int_{-1}^{1} (1-x^2) P_m'(x) P_n'(x)\, dx,$$

where $P_m(x)$ is a Legendre polynomial of order m.

22.17 Determine the minimum value that the integral

$$J = \int_0^1 [x^4(y'')^2 + 4x^2(y')^2]\, dx$$

can have, given that y is not singular at $x = 0$ and that $y(1) = y'(1) = 1$. Assume that the Euler–Lagrange equation gives the lower limit, and verify retrospectively that your solution makes the first term on the LHS of equation (22.15) vanish.

22.18 Show that $y'' - xy + \lambda x^2 y = 0$ has a solution for which $y(0) = y(1) = 0$ and $\lambda \leq 147/4$.

22.19 Find an appropriate, but simple, trial function and use it to estimate the lowest eigenvalue λ_0 of Stokes' equation,

$$\frac{d^2y}{dx^2} + \lambda x y = 0, \qquad \text{with } y(0) = y(\pi) = 0.$$

Explain why your estimate must be strictly greater than λ_0.

22.20 Estimate the lowest eigenvalue, λ_0, of the equation

$$\frac{d^2y}{dx^2} - x^2 y + \lambda y = 0, \qquad y(-1) = y(1) = 0,$$

using a quadratic trial function.

22.21 A drumskin is stretched across a fixed circular rim of radius a. Small transverse vibrations of the skin have an amplitude $z(\rho, \phi, t)$ that satisfies

$$\nabla^2 z = \frac{1}{c^2}\frac{\partial^2 z}{\partial t^2}$$

in plane polar coordinates. For a normal mode independent of azimuth, $z = Z(\rho)\cos\omega t$, find the differential equation satisfied by $Z(\rho)$. By using a trial function of the form $a^\nu - \rho^\nu$, with adjustable parameter ν, obtain an estimate for the lowest normal mode frequency.

[The exact answer is $(5.78)^{1/2}c/a$.]

22.22 Consider the problem of finding the lowest eigenvalue, λ_0, of the equation

$$(1+x^2)\frac{d^2y}{dx^2} + 2x\frac{dy}{dx} + \lambda y = 0, \qquad y(\pm 1) = 0.$$

(a) Recast the problem in variational form, and derive an approximation λ_1 to λ_0 by using the trial function $y_1(x) = 1 - x^2$.

(b) Show that an improved estimate λ_2 is obtained by using $y_2(x) = \cos(\pi x/2)$.

(c) Prove that the estimate $\lambda(\gamma)$ obtained by taking $y_1(x) + \gamma y_2(x)$ as the trial function is

$$\lambda(\gamma) = \frac{64/15 + 64\gamma/\pi - 384\gamma/\pi^3 + (\pi^2/3 + 1/2)\gamma^2}{16/15 + 64\gamma/\pi^3 + \gamma^2}.$$

Investigate $\lambda(\gamma)$ numerically as γ is varied, or, more simply, show that $\lambda(-1.80) = 3.668$, an improvement on both λ_1 and λ_2.

22.23 For the boundary conditions given below, obtain a functional $\Lambda(y)$ whose stationary values give the eigenvalues of the equation

$$(1+x)\frac{d^2y}{dx^2} + (2+x)\frac{dy}{dx} + \lambda y = 0, \qquad y(0) = 0,\ y'(2) = 0.$$

Derive an approximation to the lowest eigenvalue λ_0 using the trial function $y(x) = xe^{-x/2}$. For what value(s) of γ would

$$y(x) = xe^{-x/2} + \beta \sin \gamma x$$

be a suitable trial function for attempting to obtain an improved estimate of λ_0?

22.24 This is an alternative approach to the example in section 22.8. Using the notation of that section, the expectation value of the energy of the state ψ is given by $\int \psi^* H\psi \, dv$. Denote the eigenfunctions of H by ψ_i, so that $H\psi_i = E_i\psi_i$, and, since H is self-adjoint (Hermitian), $\int \psi_j^* \psi_i \, dv = \delta_{ij}$.

(a) By writing any function ψ as $\sum c_j\psi_j$ and following an argument similar to that in section 22.7, show that

$$E = \frac{\int \psi^* H\psi \, dv}{\int \psi^* \psi \, dv} \geq E_0,$$

the energy of the lowest state. This is the Rayleigh–Ritz principle.

(b) Using the same trial function as in section 22.8, $\psi = \exp(-\alpha x^2)$, show that the same result is obtained.

22.25 This is an extension to section 22.8 and the previous question. With the ground-state (i.e. the lowest-energy) wavefunction as $\exp(-\alpha x^2)$, take as a trial function the orthogonal wave function $x^{2n+1}\exp(-\alpha x^2)$, using the integer n as a variable parameter. Use either Sturm–Liouville theory or the Rayleigh–Ritz principle to show that the energy of the second lowest state of a quantum harmonic oscillator is $\leq 3\hbar\omega/2$.

22.26 The Hamiltonian H for the hydrogen atom is

$$-\frac{\hbar^2}{2m}\nabla^2 - \frac{q^2}{4\pi\epsilon_0 r}.$$

For a spherically symmetric state, as may be assumed for the ground state, the only relevant part of ∇^2 is that involving differentiation with respect to r.

(a) Define the integrals J_n by

$$J_n = \int_0^\infty r^n e^{-2\beta r} \, dr$$

and show that, for a trial wavefunction of the form $\exp(-\beta r)$ with $\beta > 0$, $\int \psi^* H\psi \, dv$ and $\int \psi^* \psi \, dv$ (see exercise 22.24(a)) can be expressed as $aJ_1 - bJ_2$ and cJ_2 respectively, where a, b and c are factors which you should determine.

(b) Show that the estimate of E is minimised when $\beta = mq^2/(4\pi\epsilon_0\hbar^2)$.

(c) Hence find an upper limit for the ground-state energy of the hydrogen atom. In fact, $\exp(-\beta r)$ is the correct form for the wavefunction and the limit gives the actual value.

22.27 The upper and lower surfaces of a film of liquid, which has surface energy per unit area (surface tension) γ and density ρ, have equations $z = p(x)$ and $z = q(x)$, respectively. The film has a given volume V (per unit depth in the y-direction) and lies in the region $-L < x < L$, with $p(0) = q(0) = p(L) = q(L) = 0$. The

total energy (per unit depth) of the film consists of its surface energy and its gravitational energy, and is expressed by

$$E = \tfrac{\rho g}{2}\int_{-L}^{L}(p^2 - q^2)\,dx + \gamma\int_{-L}^{L}\left[(1+p'^2)^{1/2} + (1+q'^2)^{1/2}\right]\,dx.$$

(a) Express V in terms of p and q.
(b) Show that, if the total energy is minimised, p and q must satisfy

$$\frac{p'^2}{(1+p'^2)^{1/2}} - \frac{q'^2}{(1+q'^2)^{1/2}} = \text{constant}.$$

(c) As an approximate solution, consider the equations

$$p = a(L - |x|), \qquad q = b(L - |x|),$$

where a and b are sufficiently small that a^3 and b^3 can be neglected compared with unity. Find the values of a and b that minimise E.

22.28 A particle of mass m moves in a one-dimensional potential well of the form

$$V(x) = -\mu\frac{\hbar^2\alpha^2}{m}\text{sech}^{\,2}\alpha x,$$

where μ and α are positive constants. As in exercise 22.26, the expectation value $\langle E\rangle$ of the energy of the system is $\int \psi^* H\psi\,dx$, where the self-adjoint operator H is given by $-(\hbar^2/2m)d^2/dx^2 + V(x)$. Using trial wavefunctions of the form $y = A\,\text{sech}\,\beta x$, show the following:

(a) for $\mu = 1$, there is an exact eigenfunction of H, with a corresponding $\langle E\rangle$ of half of the maximum depth of the well;
(b) for $\mu = 6$, the 'binding energy' of the ground state is at least $10\hbar^2\alpha^2/(3m)$.

[You will find it useful to note that for $u, v \geq 0$, $\text{sech}\,u\,\text{sech}\,v \geq \text{sech}\,(u+v)$.]

22.29 The Sturm–Liouville equation can be extended to two independent variables, x and z, with little modification. In equation (22.22), y'^2 is replaced by $(\nabla y)^2$ and the integrals of the various functions of $y(x,z)$ become two-dimensional, i.e. the infinitesimal is $dx\,dz$.

The vibrations of a trampoline 4 units long and 1 unit wide satisfy the equation

$$\nabla^2 y + k^2 y = 0.$$

By taking the simplest possible permissible polynomial as a trial function, show that the lowest mode of vibration has $k^2 \leq 10.63$ and, by direct solution, that the actual value is 10.49.

22.10 Hints and answers

22.1 Note that the integrand, $2\pi\rho^{1/2}(1+\rho'^2)^{1/2}$, does not contain z explicitly.

22.3 $I = \int n(r)[r^2 + (dr/d\phi)^2]^{1/2}\,d\phi$. Take axes such that $\phi = 0$ when $r = \infty$.
If $\beta = (\pi - \text{deviation angle})/2$ then $\beta = \phi$ at $r = a$, and the equation reduces to

$$\frac{\beta}{(a^2+\alpha^2)^{1/2}} = \int_{-\infty}^{\infty}\frac{dr}{r(r^2-a^2)^{1/2}},$$

which can be evaluated by putting $r = a(y + y^{-1})/2$, or successively $r = a\cosh\psi$, $y = \exp\psi$ to yield a deviation of $\pi[(a^2+\alpha^2)^{1/2} - a]/a$.

22.5 (a) $\partial x/\partial t = 0$ and so $\dot{x} = \sum_i \dot{q}_i \partial x/\partial q_i$; (b) use

$$\sum_i \dot{q}_i \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_i}\right) = \frac{d}{dt}(2T) - \sum_i \ddot{q}_i \frac{\partial T}{\partial \dot{q}_i}.$$

22.7 Use result (22.8); $\beta^2 = 1 + \alpha^2$.
Put $\rho = uc$ to obtain $d\theta/du = \beta/[u(u^2-1)^{1/2}]$. Remember that $\cos^{-1}$ is a multivalued function; $\rho(\theta) = [R\cos(\theta_0/\beta)]/[\cos(\theta/\beta)]$.

22.9 $-\lambda y'(1-y'^2)^{-1/2} = 2gP(s)$, $y = y(s)$, $P(s) = \int_0^s \rho(s')\,ds'$. The solution, $y = -a\cos(s/a)$, and $2P(\pi a/4) = M$ together give $\lambda = -gM$. The required $\rho(s)$ is given by $[M/(2a)]\sec^2(s/a)$.

22.11 Note that the ϕ E–L equation is automatically satisfied if $v \neq v(\phi)$. $A = 1/a$.

22.13 Circle is $\lambda^2 x^2 + [\lambda y + (1-\lambda^2 b^2)^{1/2}]^2 = 1$. Use the fact that $\int y\,dx = V/h$ to determine the condition on λ.

22.15 Denoting $(ds)^2/(dt)^2$ by f^2, the Euler–Lagrange equation for ϕ gives $r^2\dot{\phi} = Af$, where A corresponds to the angular momentum of the particle. Use the result of exercise 22.10 to obtain $c^2 - (2GM/r) = Bf$, where, to first order in small quantities,

$$cB = c^2 - \frac{GM}{r} + \frac{1}{2}(\dot{r}^2 + r^2\dot{\phi}^2),$$

which reads 'total energy = rest mass + gravitational energy + radial and azimuthal kinetic energy'.

22.17 Convert the equation to the usual form, by writing $y'(x) = u(x)$, and obtain $x^2u'' + 4xu' - 4u = 0$ with general solution $Ax^{-4} + Bx$. Integrating a second time and using the boundary conditions gives $y(x) = (1+x^2)/2$ and $J = 1$; $\eta(1) = 0$, since $y'(1)$ is fixed, and $\partial F/\partial u' = 2x^4u' = 0$ at $x = 0$.

22.19 Using $y = \sin x$ as a trial function shows that $\lambda_0 \leq 2/\pi$. The estimate must be $> \lambda_0$ since the trial function does not satisfy the original equation.

22.21 $Z'' + \rho^{-1}Z' + (\omega/c)^2 Z = 0$, with $Z(a) = 0$ and $Z'(0) = 0$; this is an SL equation with $p = \rho$, $q = 0$ and weight function ρ/c^2. Estimate of $\omega^2 = [c^2v/(2a^2)][0.5 - 2(v+2)^{-1} + (2v+2)^{-1}]^{-1}$, which minimises to $c^2(2+\sqrt{2})^2/(2a^2) = 5.83c^2/a^2$ when $v = \sqrt{2}$.

22.23 Note that the original equation is not self-adjoint; it needs an integrating factor of e^x. $\Lambda(y) = [\int_0^2 (1+x)e^x y'^2\,dx]/[\int_0^2 e^x y^2\,dx]$; $\lambda_0 \leq 3/8$. Since $y'(2)$ must equal 0, $\gamma = (\pi/2)(n + \frac{1}{2})$ for some integer n.

22.25 $E_1 \leq (\hbar\omega/2)(8n^2 + 12n + 3)/(4n+1)$, which has a minimum value $3\hbar\omega/2$ when integer $n = 0$.

22.27 (a) $V = \int_{-L}^{L} (p-q)\,dx$. (c) Use $V = (a-b)L^2$ to eliminate b from the expression for E; now the minimisation is with respect to a alone. The values for a and b are $\pm V/(2L^2) - V\rho g/(6\gamma)$.

22.29 The SL equation has $p = 1$, $q = 0$, and $\rho = 1$.
Use $u(x,z) = x(4-x)z(1-z)$ as a trial function; numerator = 1088/90, denominator = 512/450. Direct solution $k^2 = 17\pi^2/16$.

23

Integral equations

It is not unusual in the analysis of a physical system to encounter an equation in which an unknown but required function $y(x)$, say, appears under an integral sign. Such an equation is called an *integral equation*, and in this chapter we discuss several methods for solving the more straightforward examples of such equations.

Before embarking on our discussion of methods for solving various integral equations, we begin with a warning that many of the integral equations met in practice cannot be solved by the elementary methods presented here but must instead be solved numerically, usually on a computer. Nevertheless, the regular occurrence of several simple types of integral equation that may be solved analytically is sufficient reason to explore these equations more fully.

We shall begin this chapter by discussing how a differential equation can be transformed into an integral equation and by considering the most common types of linear integral equation. After introducing the operator notation and considering the existence of solutions for various types of equation, we go on to discuss elementary methods of obtaining closed-form solutions of simple integral equations. We then consider the solution of integral equations in terms of infinite series and conclude by discussing the properties of integral equations with Hermitian kernels, i.e. those in which the integrands have particular symmetry properties.

23.1 Obtaining an integral equation from a differential equation

Integral equations occur in many situations, partly because we may always rewrite a differential equation as an integral equation. It is sometimes advantageous to make this transformation, since questions concerning the existence of a solution are more easily answered for integral equations (see section 23.3), and, furthermore, an integral equation can incorporate automatically any boundary conditions on the solution.

We shall illustrate the principles involved by considering the differential equation

$$y''(x) = f(x, y), \tag{23.1}$$

where $f(x, y)$ can be any function of x and y but not of $y'(x)$. Equation (23.1) thus represents a large class of linear and non-linear second-order differential equations.

We can convert (23.1) into the corresponding integral equation by first integrating with respect to x to obtain

$$y'(x) = \int_0^x f(z, y(z))\, dz \ + \ c_1.$$

Integrating once more, we find

$$y(x) = \int_0^x du \int_0^u f(z, y(z))\, dz \ + \ c_1 x \ + \ c_2.$$

Provided we do not change the region in the uz-plane over which the double integral is taken, we can reverse the order of the two integrations. Changing the integration limits appropriately, we find

$$y(x) = \int_0^x f(z, y(z))\, dz \int_z^x du \ + \ c_1 x \ + \ c_2 \tag{23.2}$$

$$= \int_0^x (x - z) f(z, y(z))\, dz \ + \ c_1 x \ + \ c_2; \tag{23.3}$$

this is a non-linear (for general $f(x, y)$) *Volterra* integral equation.

It is straightforward to incorporate any boundary conditions on the solution $y(x)$ by fixing the constants c_1 and c_2 in (23.3). For example, we might have the one-point boundary condition $y(0) = a$ and $y'(0) = b$, for which it is clear that we must set $c_1 = b$ and $c_2 = a$.

23.2 Types of integral equation

From (23.3), we can see that even a relatively simple differential equation such as (23.1) can lead to a corresponding integral equation that is non-linear. In this chapter, however, we will restrict our attention to *linear* integral equations, which have the general form

$$g(x)y(x) = f(x) + \lambda \int_a^b K(x, z)y(z)\, dz. \tag{23.4}$$

In (23.4), $y(x)$ is the unknown function, while the functions $f(x)$, $g(x)$ and $K(x, z)$ are assumed known. $K(x, z)$ is called the *kernel* of the integral equation. The integration limits a and b are also assumed known, and may be constants or functions of x, and λ is a known constant or parameter.

In fact, we shall be concerned with various special cases of (23.4), which are known by particular names. Firstly, if $g(x) = 0$ then the unknown function $y(x)$ appears only under the integral sign, and (23.4) is called a linear integral equation *of the first kind*. Alternatively, if $g(x) = 1$, so that $y(x)$ appears twice, once inside the integral and once outside, then (23.4) is called a linear integral equation *of the second kind*. In either case, if $f(x) = 0$ the equation is called *homogeneous*, otherwise *inhomogeneous*.

We can distinguish further between different types of integral equation by the form of the integration limits a and b. If these limits are fixed constants then the equation is called a *Fredholm* equation. If, however, the upper limit $b = x$ (i.e. it is variable) then the equation is called a *Volterra* equation; such an equation is analogous to one with fixed limits but for which the kernel $K(x, z) = 0$ for $z > x$. Finally, we note that any equation for which either (or both) of the integration limits is infinite, or for which $K(x, z)$ becomes infinite in the range of integration, is called a *singular* integral equation.

23.3 Operator notation and the existence of solutions

There is a close correspondence between linear integral equations and the matrix equations discussed in chapter 8. However, the former involve linear, integral relations between functions in an infinite-dimensional function space (see chapter 17), whereas the latter specify linear relations among vectors in a finite-dimensional vector space.

Since we are restricting our attention to linear integral equations, it will be convenient to introduce the linear integral operator $\mathcal{K}$, whose action on an arbitrary function y is given by

$$\mathcal{K}y = \int_a^b K(x, z)y(z)\,dz. \tag{23.5}$$

This is analogous to the introduction in chapters 16 and 17 of the notation $\mathcal{L}$ to describe a linear differential operator. Furthermore, we may define the Hermitian conjugate $\mathcal{K}^\dagger$ by

$$\mathcal{K}^\dagger y = \int_a^b K^*(z, x)y(z)\,dz,$$

where the asterisk denotes complex conjugation and we have reversed the order of the arguments in the kernel.

It is clear from (23.5) that $\mathcal{K}$ is indeed linear. Moreover, since $\mathcal{K}$ operates on the infinite-dimensional space of (reasonable) functions, we may make an obvious analogy with matrix equations and consider the action of $\mathcal{K}$ on a function f as that of a matrix on a column vector (both of infinite dimension).

When written in operator form, the integral equations discussed in the previous section resemble equations familiar from linear algebra. For example, the

inhomogeneous Fredholm equation of the first kind may be written as

$$0 = f + \lambda \mathcal{K} y,$$

which has the unique solution $y = -\mathcal{K}^{-1} f/\lambda$, provided that $f \neq 0$ and the inverse operator $\mathcal{K}^{-1}$ exists.

Similarly, we may write the corresponding Fredholm equation of the second kind as

$$y = f + \lambda \mathcal{K} y. \tag{23.6}$$

In the homogeneous case, where $f = 0$, this reduces to $y = \lambda \mathcal{K} y$, which is reminiscent of an eigenvalue problem in linear algebra (except that λ appears on the other side of the equation) and, similarly, only has solutions for at most a countably infinite set of *eigenvalues* λ_i. The corresponding solutions y_i are called the eigenfunctions.

In the inhomogeneous case ($f \neq 0$), the solution to (23.6) can be written symbolically as

$$y = (1 - \lambda \mathcal{K})^{-1} f,$$

again provided that the inverse operator exists. It may be shown that, in general, (23.6) does possess a unique solution if $\lambda \neq \lambda_i$, i.e. when λ does not equal one of the eigenvalues of the corresponding homogeneous equation.

When λ does equal one of these eigenvalues, (23.6) may have either many solutions or no solution at all, depending on the form of f. If the function f is orthogonal to *every* eigenfunction of the equation

$$g = \lambda^* \mathcal{K}^\dagger g \tag{23.7}$$

that belongs to the eigenvalue λ^*, i.e.

$$\langle g | f \rangle = \int_a^b g^*(x) f(x)\, dx = 0$$

for every function g obeying (23.7), then it can be shown that (23.6) has many solutions. Otherwise the equation has no solution. These statements are discussed further in section 23.7, for the special case of integral equations with Hermitian kernels, i.e. those for which $\mathcal{K} = \mathcal{K}^\dagger$.

23.4 Closed-form solutions

In certain very special cases, it may be possible to obtain a closed-form solution of an integral equation. The reader should realise, however, when faced with an integral equation, that in general it will not be soluble by the simple methods presented in this section but must instead be solved using (numerical) iterative methods, such as those outlined in section 23.5.

23.4.1 Separable kernels

The most straightforward integral equations to solve are Fredholm equations with *separable* (or *degenerate*) kernels. A kernel is separable if it has the form

$$K(x,z) = \sum_{i=1}^{n} \phi_i(x)\psi_i(z), \tag{23.8}$$

where $\phi_i(x)$ are $\psi_i(z)$ are respectively functions of x only and of z only and the number of terms in the sum, n, is finite.

Let us consider the solution of the (inhomogeneous) Fredholm equation of the second kind,

$$y(x) = f(x) + \lambda \int_a^b K(x,z)y(z)\,dz, \tag{23.9}$$

which has a separable kernel of the form (23.8). Writing the kernel in its separated form, the functions $\phi_i(x)$ may be taken outside the integral over z to obtain

$$y(x) = f(x) + \lambda \sum_{i=1}^{n} \phi_i(x) \int_a^b \psi_i(z)y(z)\,dz.$$

Since the integration limits a and b are constant for a Fredholm equation, the integral over z in each term of the sum is just a constant. Denoting these constants by

$$c_i = \int_a^b \psi_i(z)y(z)\,dz, \tag{23.10}$$

the solution to (23.9) is found to be

$$y(x) = f(x) + \lambda \sum_{i=1}^{n} c_i\phi_i(x), \tag{23.11}$$

where the constants c_i can be evalutated by substituting (23.11) into (23.10).

►*Solve the integral equation*

$$y(x) = x + \lambda \int_0^1 (xz + z^2)y(z)\,dz. \tag{23.12}$$

The kernel for this equation is $K(x,z) = xz + z^2$, which is clearly separable, and using the notation in (23.8) we have $\phi_1(x) = x$, $\phi_2(x) = 1$, $\psi_1(z) = z$ and $\psi_2(z) = z^2$. From (23.11) the solution to (23.12) has the form

$$y(x) = x + \lambda(c_1x + c_2),$$

where the constants c_1 and c_2 are given by (23.10) as

$$c_1 = \int_0^1 z[z + \lambda(c_1z + c_2)]\,dz = \tfrac{1}{3} + \tfrac{1}{3}\lambda c_1 + \tfrac{1}{2}\lambda c_2,$$

$$c_2 = \int_0^1 z^2[z + \lambda(c_1z + c_2)]\,dz = \tfrac{1}{4} + \tfrac{1}{4}\lambda c_1 + \tfrac{1}{3}\lambda c_2.$$

These two simultaneous linear equations may be straightforwardly solved for c_1 and c_2 to give

$$c_1 = \frac{24+\lambda}{72-48\lambda-\lambda^2} \qquad \text{and} \qquad c_2 = \frac{18}{72-48\lambda-\lambda^2},$$

so that the solution to (23.12) is

$$y(x) = \frac{(72-24\lambda)x + 18\lambda}{72-48\lambda-\lambda^2}. \blacktriangleleft$$

In the above example, we see that (23.12) has a (finite) unique solution provided that λ is not equal to either root of the quadratic in the denominator of $y(x)$. The roots of this quadratic are in fact the *eigenvalues* of the corresponding homogeneous equation, as mentioned in the previous section. In general, if the separable kernel contains n terms, as in (23.8), there will be n such eigenvalues, although they may not all be different.

Kernels consisting of trigonometric (or hyperbolic) functions of sums or differences of x and z are also often separable.

►*Find the eigenvalues and corresponding eigenfunctions of the homogeneous Fredholm equation*

$$y(x) = \lambda \int_0^{\pi} \sin(x+z)\, y(z)\, dz. \tag{23.13}$$

The kernel of this integral equation can be written in separated form as

$$K(x,z) = \sin(x+z) = \sin x \cos z + \cos x \sin z,$$

so, comparing with (23.8), we have $\phi_1(x) = \sin x$, $\phi_2(x) = \cos x$, $\psi_1(z) = \cos z$ and $\psi_2(z) = \sin z$.

Thus, from (23.11), the solution to (23.13) has the form

$$y(x) = \lambda(c_1 \sin x + c_2 \cos x),$$

where the constants c_1 and c_2 are given by

$$c_1 = \lambda \int_0^{\pi} \cos z\,(c_1 \sin z + c_2 \cos z)\, dz = \frac{\lambda\pi}{2} c_2, \tag{23.14}$$

$$c_2 = \lambda \int_0^{\pi} \sin z\,(c_1 \sin z + c_2 \cos z)\, dz = \frac{\lambda\pi}{2} c_1. \tag{23.15}$$

Combining these two equations we find $c_1 = (\lambda\pi/2)^2 c_1$, and, assuming that $c_1 \neq 0$, this gives $\lambda = \pm 2/\pi$, the two eigenvalues of the integral equation (23.13).

By substituting each of the eigenvalues back into (23.14) and (23.15), we find that the eigenfunctions corresponding to the eigenvalues $\lambda_1 = 2/\pi$ and $\lambda_2 = -2/\pi$ are given respectively by

$$y_1(x) = A(\sin x + \cos x) \qquad \text{and} \qquad y_2(x) = B(\sin x - \cos x), \tag{23.16}$$

where A and B are arbitrary constants. ◄

23.4.2 Integral transform methods

If the kernel of an integral equation can be written as a function of the difference $x - z$ of its two arguments, then it is called a *displacement* kernel. An integral equation having such a kernel, and which also has the integration limits $-\infty$ to ∞, may be solved by the use of Fourier transforms (chapter 13).

If we consider the following integral equation with a displacement kernel,

$$y(x) = f(x) + \lambda \int_{-\infty}^{\infty} K(x - z)y(z)\,dz, \tag{23.17}$$

the integral over z clearly takes the form of a convolution (see chapter 13). Therefore, Fourier-transforming (23.17) and using the convolution theorem, we obtain

$$\tilde{y}(k) = \tilde{f}(k) + \sqrt{2\pi}\lambda\tilde{K}(k)\tilde{y}(k),$$

which may be rearranged to give

$$\tilde{y}(k) = \frac{\tilde{f}(k)}{1 - \sqrt{2\pi}\lambda\tilde{K}(k)}. \tag{23.18}$$

Taking the inverse Fourier transform, the solution to (23.17) is given by

$$y(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\tilde{f}(k)\exp(ikx)}{1 - \sqrt{2\pi}\lambda\tilde{K}(k)}\,dk.$$

If we can perform this inverse Fourier transformation then the solution can be found explicitly; otherwise it must be left in the form of an integral.

►*Find the Fourier transform of the function*

$$g(x) = \begin{cases} 1 & \text{if } |x| \le a, \\ 0 & \text{if } |x| > a. \end{cases}$$

Hence find an explicit expression for the solution of the integral equation

$$y(x) = f(x) + \lambda \int_{-\infty}^{\infty} \frac{\sin(x - z)}{x - z} y(z)\,dz. \tag{23.19}$$

Find the solution for the special case $f(x) = (\sin x)/x$.

The Fourier transform of $g(x)$ is given directly by

$$\tilde{g}(k) = \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} \exp(-ikx)\,dx = \left[\frac{1}{\sqrt{2\pi}} \frac{\exp(-ikx)}{(-ik)}\right]_{-a}^{a} = \sqrt{\frac{2}{\pi}} \frac{\sin ka}{k}. \tag{23.20}$$

The kernel of the integral equation (23.19) is $K(x - z) = [\sin(x - z)]/(x - z)$. Using (23.20), it is straightforward to show that the Fourier transform of the kernel is

$$\tilde{K}(k) = \begin{cases} \sqrt{\pi/2} & \text{if } |k| \le 1, \\ 0 & \text{if } |k| > 1. \end{cases} \tag{23.21}$$

Thus, using (23.18), we find the Fourier transform of the solution to be

$$\tilde{y}(k) = \begin{cases} \tilde{f}(k)/(1-\pi\lambda) & \text{if } |k| \le 1, \\ \tilde{f}(k) & \text{if } |k| > 1. \end{cases} \tag{23.22}$$

Inverse Fourier-transforming, and writing the result in a slightly more convenient form, the solution to (23.19) is given by

$$\begin{aligned} y(x) &= f(x) + \left(\frac{1}{1-\pi\lambda} - 1\right) \frac{1}{\sqrt{2\pi}} \int_{-1}^{1} \tilde{f}(k) \exp(ikx)\, dk \\ &= f(x) + \frac{\pi\lambda}{1-\pi\lambda} \frac{1}{\sqrt{2\pi}} \int_{-1}^{1} \tilde{f}(k) \exp(ikx)\, dk. \end{aligned} \tag{23.23}$$

It is clear from (23.22) that when $\lambda = 1/\pi$, which is the only eigenvalue of the corresponding homogeneous equation to (23.19), the solution becomes infinite, as we would expect.

For the special case $f(x) = (\sin x)/x$, the Fourier transform $\tilde{f}(k)$ is identical to that in (23.21), and the solution (23.23) becomes

$$\begin{aligned} y(x) &= \frac{\sin x}{x} + \left(\frac{\pi\lambda}{1-\pi\lambda}\right) \frac{1}{\sqrt{2\pi}} \int_{-1}^{1} \sqrt{\frac{\pi}{2}} \exp(ikx)\, dk \\ &= \frac{\sin x}{x} + \left(\frac{\pi\lambda}{1-\pi\lambda}\right) \frac{1}{2} \left[\frac{\exp(ikx)}{ix}\right]_{k=-1}^{k=1} \\ &= \frac{\sin x}{x} + \left(\frac{\pi\lambda}{1-\pi\lambda}\right) \frac{\sin x}{x} = \left(\frac{1}{1-\pi\lambda}\right) \frac{\sin x}{x}. \end{aligned}$$ ◀

If, instead, the integral equation (23.17) had integration limits 0 and x (so making it a Volterra equation) then its solution could be found, in a similar way, by using the convolution theorem for Laplace transforms (see chapter 13). We would find

$$\bar{y}(s) = \frac{\bar{f}(s)}{1 - \lambda \bar{K}(s)},$$

where s is the Laplace transform variable. Often one may use the dictionary of Laplace transforms given in table 13.1 to invert this equation and find the solution $y(x)$. In general, however, the evaluation of inverse Laplace transform integrals is difficult, since (in principle) it requires a contour integration; see chapter 24.

As a final example of the use of Fourier transforms in solving integral equations, we mention equations that have integration limits $-\infty$ and ∞ and a kernel of the form

$$K(x, z) = \exp(-ixz).$$

Consider, for example, the inhomogeneous Fredholm equation

$$y(x) = f(x) + \lambda \int_{-\infty}^{\infty} \exp(-ixz)\, y(z)\, dz. \tag{23.24}$$

The integral over z is clearly just (a multiple of) the Fourier transform of $y(z)$,

so we can write

$$y(x) = f(x) + \sqrt{2\pi}\lambda\tilde{y}(x). \tag{23.25}$$

If we now take the Fourier transform of (23.25) but continue to denote the independent variable by x (i.e. rather than k, for example), we obtain

$$\tilde{y}(x) = \tilde{f}(x) + \sqrt{2\pi}\lambda y(-x). \tag{23.26}$$

Substituting (23.26) into (23.25) we find

$$y(x) = f(x) + \sqrt{2\pi}\lambda\left[\tilde{f}(x) + \sqrt{2\pi}\lambda y(-x)\right],$$

but on making the change $x \to -x$ and substituting back in for $y(-x)$, this gives

$$y(x) = f(x) + \sqrt{2\pi}\lambda\tilde{f}(x) + 2\pi\lambda^2\left[f(-x) + \sqrt{2\pi}\lambda\tilde{f}(-x) + 2\pi\lambda^2 y(x)\right].$$

Thus the solution to (23.24) is given by

$$y(x) = \frac{1}{1-(2\pi)^2\lambda^4}\left[f(x) + (2\pi)^{1/2}\lambda\tilde{f}(x) + 2\pi\lambda^2 f(-x) + (2\pi)^{3/2}\lambda^3\tilde{f}(-x)\right]. \tag{23.27}$$

Clearly, (23.24) possesses a unique solution provided $\lambda \neq \pm 1/\sqrt{2\pi}$ or $\pm i/\sqrt{2\pi}$; these are easily shown to be the eigenvalues of the corresponding homogeneous equation (for which $f(x) \equiv 0$).

►*Solve the integral equation*

$$y(x) = \exp\left(-\frac{x^2}{2}\right) + \lambda\int_{-\infty}^{\infty}\exp(-ixz)\,y(z)\,dz, \tag{23.28}$$

where λ is a real constant. Show that the solution is unique unless λ has one of two particular values. Does a solution exist for either of these two values of λ?

Following the argument given above, the solution to (23.28) is given by (23.27) with $f(x) = \exp(-x^2/2)$. In order to write the solution explicitly, however, we must calculate the Fourier transform of $f(x)$. Using equation (13.7), we find $\tilde{f}(k) = \exp(-k^2/2)$, from which we note that $f(x)$ has the special property that its functional form is identical to that of its Fourier transform. Thus, the solution to (23.28) is given by

$$y(x) = \frac{1}{1-(2\pi)^2\lambda^4}\left[1 + (2\pi)^{1/2}\lambda + 2\pi\lambda^2 + (2\pi)^{3/2}\lambda^3\right]\exp\left(-\frac{x^2}{2}\right). \tag{23.29}$$

Since λ is restricted to be real, the solution to (23.28) will be unique unless $\lambda = \pm 1/\sqrt{2\pi}$, at which points (23.29) becomes infinite. In order to find whether solutions exist for either of these values of λ we must return to equations (23.25) and (23.26).

Let us first consider the case $\lambda = +1/\sqrt{2\pi}$. Putting this value into (23.25) and (23.26), we obtain

$$y(x) = f(x) + \tilde{y}(x), \tag{23.30}$$

$$\tilde{y}(x) = \tilde{f}(x) + y(-x). \tag{23.31}$$

Substituting (23.31) into (23.30) we find

$$y(x) = f(x) + \tilde{f}(x) + y(-x),$$

but on changing x to $-x$ and substituting back in for $y(-x)$, this gives

$$y(x) = f(x) + \tilde{f}(x) + f(-x) + \tilde{f}(-x) + y(x).$$

Thus, in order for a solution to exist, we require that the function $f(x)$ obeys

$$f(x) + \tilde{f}(x) + f(-x) + \tilde{f}(-x) = 0.$$

This is satisfied if $f(x) = -\tilde{f}(x)$, i.e. if the functional form of $f(x)$ is minus the form of its Fourier transform. We may repeat this analysis for the case $\lambda = -1/\sqrt{2\pi}$, and, in a similar way, we find that this time we require $f(x) = \tilde{f}(x)$.

In our case $f(x) = \exp(-x^2/2)$, for which, as we mentioned above, $f(x) = \tilde{f}(x)$. Therefore, (23.28) possesses no solution when $\lambda = +1/\sqrt{2\pi}$ but has many solutions when $\lambda = -1/\sqrt{2\pi}$. ◄

A similar approach to the above may be taken to solve equations with kernels of the form $K(x, y) = \cos xy$ or $\sin xy$, either by considering the integral over y in each case as the real or imaginary part of the corresponding Fourier transform or by using Fourier cosine or sine transforms directly.

23.4.3 Differentiation

A closed-form solution to a Volterra equation may sometimes be obtained by differentiating the equation to obtain the corresponding differential equation, which may be easier to solve.

►*Solve the integral equation*

$$y(x) = x - \int_0^x xz^2 y(z)\, dz. \tag{23.32}$$

Dividing through by x, we obtain

$$\frac{y(x)}{x} = 1 - \int_0^x z^2 y(z)\, dz,$$

which may be differentiated with respect to x to give

$$\frac{d}{dx}\left[\frac{y(x)}{x}\right] = -x^2 y(x) = -x^3\left[\frac{y(x)}{x}\right].$$

This equation may be integrated straightforwardly, and we find

$$\ln\left[\frac{y(x)}{x}\right] = -\frac{x^4}{4} + c,$$

where c is a constant of integration. Thus the solution to (23.32) has the form

$$y(x) = Ax \exp\left(-\frac{x^4}{4}\right), \tag{23.33}$$

where A is an arbitrary constant.

Since the original integral equation (23.32) contains no arbitrary constants, neither should its solution. We may calculate the value of the constant, A, by substituting the solution (23.33) back into (23.32), from which we find $A = 1$. ◄

23.5 Neumann series

As mentioned above, most integral equations met in practice will not be of the simple forms discussed in the last section and so, in general, it is not possible to find closed-form solutions. In such cases, we might try to obtain a solution in the form of an infinite series, as we did for differential equations (see chapter 16).

Let us consider the equation

$$y(x) = f(x) + \lambda \int_a^b K(x,z)y(z)\,dz, \tag{23.34}$$

where either both integration limits are constants (for a Fredholm equation) or the upper limit is variable (for a Volterra equation). Clearly, if λ were small then a crude (but reasonable) approximation to the solution would be

$$y(x) \approx y_0(x) = f(x),$$

where $y_0(x)$ stands for our 'zeroth-order' approximation to the solution (and is not to be confused with an eigenfunction).

Substituting this crude guess under the integral sign in the original equation, we obtain what should be a better approximation:

$$y_1(x) = f(x) + \lambda \int_a^b K(x,z)y_0(z)\,dz = f(x) + \lambda \int_a^b K(x,z)f(z)\,dz,$$

which is first order in λ. Repeating the procedure once more results in the second-order approximation

$$\begin{aligned} y_2(x) &= f(x) + \lambda \int_a^b K(x,z)y_1(z)\,dz \\ &= f(x) + \lambda \int_a^b K(x,z_1)f(z_1)\,dz_1 + \lambda^2 \int_a^b dz_1 \int_a^b K(x,z_1)K(z_1,z_2)f(z_2)\,dz_2. \end{aligned}$$

It is clear that we may continue this process to obtain progressively higher-order approximations to the solution. Introducing the functions

$$\begin{aligned} K_1(x,z) &= K(x,z), \\ K_2(x,z) &= \int_a^b K(x,z_1)K(z_1,z)\,dz_1, \\ K_3(x,z) &= \int_a^b dz_1 \int_a^b K(x,z_1)K(z_1,z_2)K(z_2,z)\,dz_2, \end{aligned}$$

and so on, which obey the recurrence relation

$$K_n(x,z) = \int_a^b K(x,z_1)K_{n-1}(z_1,z)\,dz_1,$$

we may write the nth-order approximation as

$$y_n(x) = f(x) + \sum_{m=1}^{n} \lambda^m \int_a^b K_m(x,z) f(z)\, dz. \tag{23.35}$$

The solution to the original integral equation is then given by $y(x) = \lim_{n\to\infty} y_n(x)$, *provided the infinite series converges.* Using (23.35), this solution may be written as

$$y(x) = f(x) + \lambda \int_a^b R(x,z;\lambda) f(z)\, dz, \tag{23.36}$$

where the *resolvent kernel* $R(x,z;\lambda)$ is given by

$$R(x,z;\lambda) = \sum_{m=0}^{\infty} \lambda^m K_{m+1}(x,z). \tag{23.37}$$

Clearly, the resolvent kernel, and hence the series solution, will converge provided λ is sufficiently small. In fact, it may be shown that the series converges in some domain of $|\lambda|$ provided the original kernel $K(x,z)$ is bounded in such a way that

$$|\lambda|^2 \int_a^b dx \int_a^b |K(x,z)|^2\, dz < 1. \tag{23.38}$$

►*Use the Neumann series method to solve the integral equation*

$$y(x) = x + \lambda \int_0^1 xz y(z)\, dz. \tag{23.39}$$

Following the method outlined above, we begin with the crude approximation $y(x) \approx y_0(x) = x$. Substituting this under the integral sign in (23.39), we obtain the next approximation

$$y_1(x) = x + \lambda \int_0^1 xz y_0(z)\, dz = x + \lambda \int_0^1 xz^2 dz \;=\; x + \frac{\lambda x}{3},$$

Repeating the procedure once more, we obtain

$$\begin{aligned} y_2(x) &= x + \lambda \int_0^1 xz y_1(z)\, dz \\ &= x + \lambda \int_0^1 xz \left(z + \frac{\lambda z}{3}\right) dz \;=\; x + \left(\frac{\lambda}{3} + \frac{\lambda^2}{9}\right) x. \end{aligned}$$

For this simple example, it is easy to see that by continuing this process the solution to (23.39) is obtained as

$$y(x) = x + \left[\frac{\lambda}{3} + \left(\frac{\lambda}{3}\right)^2 + \left(\frac{\lambda}{3}\right)^3 + \cdots\right] x.$$

Clearly the expression in brackets is an infinite geometric series with first term $\lambda/3$ and

common ratio $\lambda/3$. Thus, *provided* $|\lambda| < 3$, this infinite series converges to the value $\lambda/(3-\lambda)$, and the solution to (23.39) is

$$y(x) = x + \frac{\lambda x}{3-\lambda} = \frac{3x}{3-\lambda}. \tag{23.40}$$

Finally, we note that the requirement that $|\lambda| < 3$ may also be derived very easily from the condition (23.38). ◄

23.6 Fredholm theory

In the previous section, we found that a solution to the integral equation (23.34) can be obtained as a Neumann series of the form (23.36), where the resolvent kernel $R(x,z;\lambda)$ is written as an infinite power series in λ. This solution is valid provided the infinite series converges.

A related, but more elegant, approach to the solution of integral equations using infinite series was found by Fredholm. We will not reproduce Fredholm's analysis here, but merely state the results we need. Essentially, *Fredholm theory* provides a formula for the resolvent kernel $R(x,z;\lambda)$ in (23.36) in terms of the ratio of two infinite series:

$$R(x,z;\lambda) = \frac{D(x,z;\lambda)}{d(\lambda)}. \tag{23.41}$$

The numerator and denominator in (23.41) are given by

$$D(x,z;\lambda) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} D_n(x,z)\lambda^n, \tag{23.42}$$

$$d(\lambda) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} d_n \lambda^n, \tag{23.43}$$

where the functions $D_n(x,z)$ and the constants d_n are found from recurrence relations as follows. We start with

$$D_0(x,z) = K(x,z) \qquad \text{and} \qquad d_0 = 1, \tag{23.44}$$

where $K(x,z)$ is the kernel of the original integral equation (23.34). The higher-order coefficients of λ in (23.43) and (23.42) are then obtained from the two recurrence relations

$$d_n = \int_a^b D_{n-1}(x,x)\,dx, \tag{23.45}$$

$$D_n(x,z) = K(x,z)d_n - n\int_a^b K(x,z_1)D_{n-1}(z_1,z)\,dz_1. \tag{23.46}$$

Although the formulae for the resolvent kernel appear complicated, they are often simple to apply. Moreover, for the Fredholm solution the power series (23.42) and (23.43) are both guaranteed to converge for all values of λ, unlike

Neumann series, which converge only if the condition (23.38) is satisfied. Thus the Fredholm method leads to a unique, non-singular solution, provided that $d(\lambda) \neq 0$. In fact, as we might suspect, the solutions of $d(\lambda) = 0$ give the eigenvalues of the homogeneous equation corresponding to (23.34), i.e. with $f(x) \equiv 0$.

► *Use Fredholm theory to solve the integral equation (23.39).*

Using (23.36) and (23.41), the solution to (23.39) can be written in the form

$$y(x) = x + \lambda \int_0^1 R(x, z; \lambda) z \, dz = x + \lambda \int_0^1 \frac{D(x, z; \lambda)}{d(\lambda)} z \, dz. \tag{23.47}$$

In order to find the form of the resolvent kernel $R(x, z; \lambda)$, we begin by setting

$$D_0(x, z) = K(x, z) = xz \qquad \text{and} \qquad d_0 = 1$$

and use the recurrence relations (23.45) and (23.46) to obtain

$$d_1 = \int_0^1 D_0(x, x) \, dx = \int_0^1 x^2 \, dx = \frac{1}{3},$$

$$D_1(x, z) = \frac{xz}{3} - \int_0^1 x z_1^2 z \, dz_1 = \frac{xz}{3} - xz \left[\frac{z_1^3}{3} \right]_0^1 = 0.$$

Applying the recurrence relations again we find that $d_n = 0$ and $D_n(x, z) = 0$ for $n > 1$. Thus, from (23.42) and (23.43), the numerator and denominator of the resolvent respectively are given by

$$D(x, z; \lambda) = xz \qquad \text{and} \qquad d(\lambda) = 1 - \frac{\lambda}{3}.$$

Substituting these expressions into (23.47), we find that the solution to (23.39) is given by

$$y(x) = x + \lambda \int_0^1 \frac{xz^2}{1 - \lambda/3} \, dz$$

$$= x + \lambda \left[\frac{x}{1 - \lambda/3} \frac{z^3}{3} \right]_0^1 = x + \frac{\lambda x}{3 - \lambda} = \frac{3x}{3 - \lambda},$$

which, as expected, is the same as the solution (23.40) found by constructing a Neumann series. ◄

23.7 Schmidt–Hilbert theory

The Schmidt–Hilbert (SH) theory of integral equations may be considered as analogous to the Sturm–Liouville (SL) theory of differential equations, discussed in chapter 17, and is concerned with the properties of integral equations with *Hermitian* kernels. An Hermitian kernel enjoys the property

$$K(x, z) = K^*(z, x), \tag{23.48}$$

and it is clear that a special case of (23.48) occurs for a real kernel that is also symmetric with respect to its two arguments.

Let us begin by considering the homogeneous integral equation

$$y = \lambda \mathcal{K} y,$$

where the integral operator $\mathcal{K}$ has an Hermitian kernel. As discussed in section 23.3, in general this equation will have solutions only for $\lambda = \lambda_i$, where the λ_i are the eigenvalues of the integral equation, the corresponding solutions y_i being the eigenfunctions of the equation.

By following similar arguments to those presented in chapter 17 for SL theory, it may be shown that the eigenvalues λ_i of an Hermitian kernel are real and that the corresponding eigenfunctions y_i belonging to different eigenvalues are orthogonal and form a complete set. If the eigenfunctions are suitably normalised, we have

$$\langle y_i | y_j \rangle = \int_a^b y_i^*(x) y_j(x)\, dx = \delta_{ij}. \tag{23.49}$$

If an eigenvalue is degenerate then the eigenfunctions corresponding to that eigenvalue can be made orthogonal by the Gram–Schmidt procedure, in a similar way to that discussed in chapter 17 in the context of SL theory.

Like SL theory, SH theory does not provide a method of obtaining the eigenvalues and eigenfunctions of any particular homogeneous integral equation with an Hermitian kernel; for this we have to turn to the methods discussed in the previous sections of this chapter. Rather, SH theory is concerned with the general properties of the solutions to such equations. Where SH theory becomes applicable, however, is in the solution of inhomogeneous integral equations with Hermitian kernels for which the eigenvalues and eigenfunctions of the corresponding homogeneous equation are already known.

Let us consider the inhomogeneous equation

$$y = f + \lambda \mathcal{K} y, \tag{23.50}$$

where $\mathcal{K} = \mathcal{K}^\dagger$ and for which we know the eigenvalues λ_i and normalised eigenfunctions y_i of the corresponding homogeneous problem. The function f may or may not be expressible solely in terms of the eigenfunctions y_i, and to accommodate this situation we write the unknown solution y as $y = f + \sum_i a_i y_i$, where the a_i are expansion coefficients to be determined.

Substituting this into (23.50), we obtain

$$f + \sum_i a_i y_i = f + \lambda \sum_i \frac{a_i y_i}{\lambda_i} + \lambda \mathcal{K} f, \tag{23.51}$$

where we have used the fact that $y_i = \lambda_i \mathcal{K} y_i$. Forming the inner product of both

sides of (23.51) with y_j, we find

$$\sum_i a_i \langle y_j | y_i \rangle = \lambda \sum_i \frac{a_i}{\lambda_i} \langle y_j | y_i \rangle + \lambda \langle y_j | \mathcal{K} f \rangle. \tag{23.52}$$

Since the eigenfunctions are orthonormal and $\mathcal{K}$ is an Hermitian operator, we have that both $\langle y_j | y_i \rangle = \delta_{ij}$ and $\langle y_j | \mathcal{K} f \rangle = \langle \mathcal{K} y_j | f \rangle = \lambda_j^{-1} \langle y_j | f \rangle$. Thus the coefficients a_j are given by

$$a_j = \frac{\lambda \lambda_j^{-1} \langle y_j | f \rangle}{1 - \lambda \lambda_j^{-1}} = \frac{\lambda \langle y_j | f \rangle}{\lambda_j - \lambda}, \tag{23.53}$$

and the solution is

$$y = f + \sum_i a_i y_i = f + \lambda \sum_i \frac{\langle y_i | f \rangle}{\lambda_i - \lambda} y_i. \tag{23.54}$$

This also shows, incidentally, that a formal representation for the resolvent kernel is

$$R(x, z; \lambda) = \sum_i \frac{y_i(x) y_i^*(z)}{\lambda_i - \lambda}. \tag{23.55}$$

If f *can* be expressed as a linear superposition of the y_i, i.e. $f = \sum_i b_i y_i$, then $b_i = \langle y_i | f \rangle$ and the solution can be written more briefly as

$$y = \sum_i \frac{b_i}{1 - \lambda \lambda_i^{-1}} y_i. \tag{23.56}$$

We see from (23.54) that the inhomogeneous equation (23.50) has a unique solution provided $\lambda \neq \lambda_i$, i.e. when λ is not equal to one of the eigenvalues of the corresponding homogeneous equation. However, if λ does equal one of the eigenvalues λ_j then, in general, the coefficients a_j become singular and no (finite) solution exists.

Returning to (23.53), we notice that even if $\lambda = \lambda_j$ a non-singular solution to the integral equation is still possible provided that the function f is orthogonal to every eigenfunction corresponding to the eigenvalue λ_j, i.e.

$$\langle y_j | f \rangle = \int_a^b y_j^*(x) f(x)\, dx = 0.$$

The following worked example illustrates the case in which f can be expressed in terms of the y_i. One in which it cannot is considered in exercise 23.14.

► *Use Schmidt–Hilbert theory to solve the integral equation*

$$y(x) = \sin(x + \alpha) + \lambda \int_0^\pi \sin(x + z) y(z)\, dz. \tag{23.57}$$

It is clear that the kernel $K(x, z) = \sin(x + z)$ is real and symmetric in x and z and is

thus Hermitian. In order to solve this inhomogeneous equation using SH theory, however, we must first find the eigenvalues and eigenfunctions of the corresponding homogeneous equation.

In fact, we have considered the solution of the corresponding homogeneous equation (23.13) already, in subsection 23.4.1, where we found that it has two eigenvalues $\lambda_1 = 2/\pi$ and $\lambda_2 = -2/\pi$, with eigenfunctions given by (23.16). The normalised eigenfunctions are

$$y_1(x) = \frac{1}{\sqrt{\pi}}(\sin x + \cos x) \quad \text{and} \quad y_2(x) = \frac{1}{\sqrt{\pi}}(\sin x - \cos x) \tag{23.58}$$

and are easily shown to obey the orthonormality condition (23.49).

Using (23.54), the solution to the inhomogeneous equation (23.57) has the form

$$y(x) = a_1 y_1(x) + a_2 y_2(x), \tag{23.59}$$

where the coefficients a_1 and a_2 are given by (23.53) with $f(x) = \sin(x + \alpha)$. Therefore, using (23.58),

$$\begin{aligned} a_1 &= \frac{1}{1 - \pi\lambda/2} \int_0^\pi \frac{1}{\sqrt{\pi}}(\sin z + \cos z)\sin(z + \alpha)\, dz &&= \frac{\sqrt{\pi}}{2 - \pi\lambda}(\cos\alpha + \sin\alpha), \\ a_2 &= \frac{1}{1 + \pi\lambda/2} \int_0^\pi \frac{1}{\sqrt{\pi}}(\sin z - \cos z)\sin(z + \alpha)\, dz &&= \frac{\sqrt{\pi}}{2 + \pi\lambda}(\cos\alpha - \sin\alpha). \end{aligned}$$

Substituting these expressions for a_1 and a_2 into (23.59) and simplifying, we find that the solution to (23.57) is given by

$$y(x) = \frac{1}{1 - (\pi\lambda/2)^2}\left[\sin(x + \alpha) + (\pi\lambda/2)\cos(x - \alpha)\right]. \blacktriangleleft$$

23.8 Exercises

23.1 Solve the integral equation

$$\int_0^\infty \cos(xv)y(v)\, dv = \exp(-x^2/2)$$

for the function $y = y(x)$ for $x > 0$. Note that for $x < 0$, $y(x)$ can be chosen as is most convenient.

23.2 Solve

$$\int_0^\infty f(t)\exp(-st)\, dt = \frac{a}{a^2 + s^2}.$$

23.3 Convert

$$f(x) = \exp x + \int_0^x (x - y)f(y)\, dy$$

into a differential equation, and hence show that its solution is

$$(\alpha + \beta x)\exp x + \gamma\, \exp(-x),$$

where α, β and γ are constants that should be determined.

23.4 Use the fact that its kernel is separable, to solve for $y(x)$ the integral equation

$$y(x) = A\cos(x + a) + \lambda \int_0^\pi \sin(x + z)y(z)\, dz.$$

[This equation is an inhomogeneous extension of the homogeneous Fredholm equation (23.13), and is similar to equation (23.57).]

23.5 Solve for $\phi(x)$ the integral equation

$$\phi(x) = f(x) + \lambda \int_0^1 \left[\left(\frac{x}{y}\right)^n + \left(\frac{y}{x}\right)^n \right] \phi(y)\, dy,$$

where $f(x)$ is bounded for $0 < x < 1$ and $-\frac{1}{2} < n < \frac{1}{2}$, expressing your answer in terms of the quantities $F_m = \int_0^1 f(y) y^m\, dy$.

(a) Give the explicit solution when $\lambda = 1$.
(b) For what values of λ are there no solutions unless $F_{\pm n}$ are in a particular ratio? What is this ratio?

23.6 Consider the inhomogeneous integral equation

$$f(x) = g(x) + \lambda \int_a^b K(x, y) f(y)\, dy,$$

for which the kernel $K(x, y)$ is real, symmetric and continuous in $a \leq x \leq b$, $a \leq y \leq b$.

(a) If λ is one of the eigenvalues λ_i of the homogeneous equation

$$f_i(x) = \lambda_i \int_a^b K(x, y) f_i(y)\, dy,$$

prove that the inhomogeneous equation can only a have non-trivial solution if $g(x)$ is orthogonal to the corresponding eigenfunction $f_i(x)$.
(b) Show that the only values of λ for which

$$f(x) = \lambda \int_0^1 xy(x + y) f(y)\, dy$$

has a non-trivial solution are the roots of the equation

$$\lambda^2 + 120\lambda - 240 = 0.$$

(c) Solve

$$f(x) = \mu x^2 + \int_0^1 2xy(x + y) f(y)\, dy.$$

23.7 The kernel of the integral equation

$$\psi(x) = \lambda \int_a^b K(x, y) \psi(y)\, dy$$

has the form

$$K(x, y) = \sum_{n=0}^{\infty} h_n(x) g_n(y),$$

where the $h_n(x)$ form a complete orthonormal set of functions over the interval $[a, b]$.

(a) Show that the eigenvalues λ_i are given by

$$|\mathsf{M} - \lambda^{-1}\mathsf{I}| = 0,$$

where M is the matrix with elements

$$M_{kj} = \int_a^b g_k(u) h_j(u)\, du.$$

If the corresponding solutions are $\psi^{(i)}(x) = \sum_{n=0}^{\infty} a_n^{(i)} h_n(x)$, find an expression for $a_n^{(i)}$.

(b) Obtain the eigenvalues and eigenfunctions over the interval $[0, 2\pi]$ if

$$K(x, y) = \sum_{n=1}^{\infty} \frac{1}{n} \cos nx \cos ny.$$

23.8 By taking its Laplace transform, and that of $x^n e^{-ax}$, obtain the explicit solution of

$$f(x) = e^{-x} \left[x + \int_0^x (x - u) e^u f(u)\, du \right].$$

Verify your answer by substitution.

23.9 For $f(t) = \exp(-t^2/2)$, use the relationships of the Fourier transforms of $f'(t)$ and $tf(t)$ to that of $f(t)$ itself to find a simple differential equation satisfied by $\tilde{f}(\omega)$, the Fourier transform of $f(t)$, and hence determine $\tilde{f}(\omega)$ to within a constant. Use this result to solve the integral equation

$$\int_{-\infty}^{\infty} e^{-t(t-2x)/2} h(t)\, dt = e^{3x^2/8}$$

for $h(t)$.

23.10 Show that the equation

$$f(x) = x^{-1/3} + \lambda \int_0^{\infty} f(y) \exp(-xy)\, dy$$

has a solution of the form $Ax^{\alpha} + Bx^{\beta}$. Determine the values of α and β, and show that those of A and B are

$$\frac{1}{1 - \lambda^2 \Gamma(\frac{1}{3})\Gamma(\frac{2}{3})} \quad \text{and} \quad \frac{\lambda \Gamma(\frac{2}{3})}{1 - \lambda^2 \Gamma(\frac{1}{3})\Gamma(\frac{2}{3})},$$

where $\Gamma(z)$ is the gamma function.

23.11 At an international 'peace' conference a large number of delegates are seated around a circular table with each delegation sitting near its allies and diametrically opposite the delegation most bitterly opposed to it. The position of a delegate is denoted by θ, with $0 \leq \theta \leq 2\pi$. The fury $f(\theta)$ felt by the delegate at θ is the sum of his own natural hostility $h(\theta)$ and the influences on him of each of the other delegates; a delegate at position ϕ contributes an amount $K(\theta - \phi) f(\phi)$. Thus

$$f(\theta) = h(\theta) + \int_0^{2\pi} K(\theta - \phi) f(\phi)\, d\phi.$$

Show that if $K(\psi)$ takes the form $K(\psi) = k_0 + k_1 \cos\psi$ then

$$f(\theta) = h(\theta) + p + q \cos\theta + r \sin\theta$$

and evaluate p, q and r. A positive value for k_1 implies that delegates tend to placate their opponents but upset their allies, whilst negative values imply that they calm their allies but infuriate their opponents. A walkout will occur if $f(\theta)$ exceeds a certain threshold value for some θ. Is this more likely to happen for positive or for negative values of k_1?

23.12 By considering functions of the form $h(x) = \int_0^x (x - y) f(y)\, dy$, show that the solution $f(x)$ of the integral equation

$$f(x) = x + \tfrac{1}{2} \int_0^1 |x - y| f(y)\, dy$$

satisfies the equation $f''(x) = f(x)$.

By examining the special cases $x = 0$ and $x = 1$, show that

$$f(x) = \frac{2}{(e+3)(e+1)}[(e+2)e^x - ee^{-x}].$$

23.13 The operator $\mathscr{M}$ is defined by

$$\mathscr{M}f(x) \equiv \int_{-\infty}^{\infty} K(x,y)f(y)\,dy,$$

where $K(x,y) = 1$ inside the square $|x| < a, |y| < a$ and $K(x,y) = 0$ elsewhere. Consider the possible eigenvalues of $\mathscr{M}$ and the eigenfunctions that correspond to them; show that the only possible eigenvalues are 0 and $2a$ and determine the corresponding eigenfunctions. Hence find the general solution of

$$f(x) = g(x) + \lambda \int_{-\infty}^{\infty} K(x,y)f(y)\,dy.$$

23.14 For the integral equation

$$y(x) = x^{-3} + \lambda \int_a^b x^2 z^2 y(z)\,dz,$$

show that the resolvent kernel is $5x^2z^2/[5 - \lambda(b^5 - a^5)]$ and hence solve the equation. For what range of λ is the solution valid?

23.15 Use Fredholm theory to show that, for the kernel

$$K(x,z) = (x+z)\exp(x-z)$$

over the interval $[0,1]$, the resolvent kernel is

$$R(x,z;\lambda) = \frac{\exp(x-z)[(x+z) - \lambda(\frac{1}{2}x + \frac{1}{2}z - xz - \frac{1}{3})]}{1 - \lambda - \frac{1}{12}\lambda^2},$$

and hence solve

$$y(x) = x^2 + 2\int_0^1 (x+z)\exp(x-z)\,y(z)\,dz,$$

expressing your answer in terms of I_n, where $I_n = \int_0^1 u^n \exp(-u)\,du$.

23.16 This exercise shows that following formal theory is not necessarily the best way to get practical results!

(a) Determine the eigenvalues $\lambda_\pm$ of the kernel $K(x,z) = (xz)^{1/2}(x^{1/2} + z^{1/2})$ and show that the corresponding eigenfunctions have the forms

$$y_\pm(x) = A_\pm(\sqrt{2}x^{1/2} \pm \sqrt{3}x),$$

where $A_\pm^2 = 5/(10 \pm 4\sqrt{6})$.

(b) Use Schmidt–Hilbert theory to solve

$$y(x) = 1 + \tfrac{5}{2}\int_0^1 K(x,z)y(z)\,dz.$$

(c) As will have been apparent, the algebra involved in the formal method used in (b) is long and error-prone, and it is in fact much more straightforward to use a trial function $1 + \alpha x^{1/2} + \beta x$. Check your answer by doing so.

23.9 Hints and answers

23.1 Define $y(-x) = y(x)$ and use the cosine Fourier transform inversion theorem; $y(x) = (2/\pi)^{1/2}\exp(-x^2/2)$.

23.3 $f''(x) - f(x) = \exp x$; $\alpha = 3/4$, $\beta = 1/2$, $\gamma = 1/4$.

23.5 (a) $\phi(x) = f(x) - (1+2n)F_n x^n - (1-2n)F_{-n}x^{-n}$. (b) There are no solutions for $\lambda = [1 \pm (1-4n^2)^{-1/2}]^{-1}$ unless $F_{\pm n} = 0$ or $F_n/F_{-n} = \mp[(1-2n)/(1+2n)]^{1/2}$.

23.7 (a) $a_n^{(i)} = \int_a^b h_n(x)\psi^{(i)}(x)\,dx$; (b) use $(1/\sqrt{\pi})\cos nx$ and $(1/\sqrt{\pi})\sin nx$; M is diagonal; eigenvalues $\lambda_k = k/\pi$ with eigenfunctions $\psi^{(k)}(x) = (1/\sqrt{\pi})\cos kx$.

23.9 $d\tilde{f}/d\omega = -\omega\tilde{f}$, leading to $\tilde{f}(\omega) = Ae^{-\omega^2/2}$. Rearrange the integral as a convolution and deduce that $\tilde{h}(\omega) = Be^{-3\omega^2/2}$; $h(t) = Ce^{-t^2/6}$, where resubstitution and Gaussian normalisation show that $C = \sqrt{2/(3\pi)}$.

23.11 $p = k_0 H/(1-2\pi k_0)$, $q = k_1 H_c/(1-\pi k_1)$ and $r = k_1 H_s/(1-\pi k_1)$, where $H = \int_0^{2\pi} h(z)\,dz$, $H_c = \int_0^{2\pi} h(z)\cos z\,dz$, and $H_s = \int_0^{2\pi} h(z)\sin z\,dz$. Positive values of $k_1 (\approx \pi^{-1})$ are most likely to cause a conference breakdown.

23.13 For eigenvalue 0 : $f(x) = 0$ for $|x| < a$ or $f(x)$ is such that $\int_{-a}^{a} f(y)dy = 0$.
For eigenvalue $2a$: $f(x) = \mu S(x,a)$ with μ a constant and $S(x,a) \equiv [H(a+x) - H(x-a)]$, where $H(z)$ is the Heaviside step function.
Take $f(x) = g(x) + cGS(x,a)$, where $G = \int_{-a}^{a} g(z)\,dz$. Show that $c = \lambda/(1-2a\lambda)$.

23.15 $y(x) = x^2 - (3I_3 x + I_2)\exp x$.

24

Complex variables

Throughout this book references have been made to results derived from the theory of complex variables. This theory thus becomes an integral part of the mathematics appropriate to physical applications. Indeed, so numerous and widespread are these applications that the whole of the next chapter is devoted to a systematic presentation of some of the more important ones. This current chapter develops the general theory on which these applications are based. The difficulty with it, from the point of view of a book such as the present one, is that the underlying basis has a distinctly pure mathematics flavour.

Thus, to adopt a comprehensive rigorous approach would involve a large amount of groundwork in analysis, for example formulating precise definitions of continuity and differentiability, developing the theory of sets and making a detailed study of boundedness. Instead, we will be selective and pursue only those parts of the formal theory that are needed to establish the results used in the next chapter and elsewhere in this book.

In this spirit, the proofs that have been adopted for some of the standard results of complex variable theory have been chosen with an eye to simplicity rather than sophistication. This means that in some cases the imposed conditions are more stringent than would be strictly necessary if more sophisticated proofs were used; where this happens the less restrictive results are usually stated as well. The reader who is interested in a fuller treatment should consult one of the many excellent textbooks on this fascinating subject.[§]

One further concession to 'hand-waving' has been made in the interests of keeping the treatment to a moderate length. In several places phrases such as 'can be made as small as we like' are used, rather than a careful treatment in terms of 'given $\epsilon > 0$, there exists a $\delta > 0$ such that'. In the authors' experience, some

[§] For example, K. Knopp, *Theory of Functions, Part I* (New York: Dover, 1945); E. G. Phillips, *Functions of a Complex Variable with Applications* 7th edn (Edinburgh: Oliver and Boyd, 1951); E. C. Titchmarsh, *The Theory of Functions* (Oxford: Oxford University Press, 1952).

students are more at ease with the former type of statement, despite its lack of precision, whilst others, those who would contemplate only the latter, are usually well able to supply it for themselves.

24.1 Functions of a complex variable

The quantity $f(z)$ is said to be a function of the complex variable z if to every value of z in a certain domain R (a region of the Argand diagram) there corresponds one or more values of $f(z)$. Stated like this $f(z)$ could be any function consisting of a real and an imaginary part, each of which is, in general, itself a function of x and y. If we denote the real and imaginary parts of $f(z)$ by u and v, respectively, then

$$f(z) = u(x, y) + iv(x, y).$$

In this chapter, however, we will be primarily concerned with functions that are single-valued, so that to each value of z there corresponds just one value of $f(z)$, and are differentiable in a particular sense, which we now discuss.

A function $f(z)$ that is single-valued in some domain R is *differentiable* at the point z in R if the *derivative*

$$f'(z) = \lim_{\Delta z \to 0} \left[\frac{f(z + \Delta z) - f(z)}{\Delta z} \right] \tag{24.1}$$

exists and is unique, in that its value does not depend upon the direction in the Argand diagram from which Δz tends to zero.

►*Show that the function $f(z) = x^2 - y^2 + i2xy$ is differentiable for all values of z.*

Considering the definition (24.1), and taking $\Delta z = \Delta x + i\Delta y$, we have

$$\begin{aligned}
&\frac{f(z + \Delta z) - f(z)}{\Delta z} \\
&\quad = \frac{(x + \Delta x)^2 - (y + \Delta y)^2 + 2i(x + \Delta x)(y + \Delta y) - x^2 + y^2 - 2ixy}{\Delta x + i\Delta y} \\
&\quad = \frac{2x\Delta x + (\Delta x)^2 - 2y\Delta y - (\Delta y)^2 + 2i(x\Delta y + y\Delta x + \Delta x\Delta y)}{\Delta x + i\Delta y} \\
&\quad = 2x + i2y + \frac{(\Delta x)^2 - (\Delta y)^2 + 2i\Delta x\Delta y}{\Delta x + i\Delta y}.
\end{aligned}$$

Now, in whatever way Δx and Δy are allowed to tend to zero (e.g. taking $\Delta y = 0$ and letting $\Delta x \to 0$ or vice versa), the last term on the RHS will tend to zero and the unique limit $2x + i2y$ will be obtained. Since z was arbitrary, $f(z)$ with $u = x^2 - y^2$ and $v = 2xy$ is differentiable at all points in the (finite) complex plane. ◄

We note that the above working can be considerably reduced by recognising that, since $z = x + iy$, we can write $f(z)$ as

$$f(z) = x^2 - y^2 + 2ixy = (x + iy)^2 = z^2.$$

We then find that

$$f'(z) = \lim_{\Delta z \to 0}\left[\frac{(z+\Delta z)^2 - z^2}{\Delta z}\right] = \lim_{\Delta z \to 0}\left[\frac{(\Delta z)^2 + 2z\Delta z}{\Delta z}\right]$$
$$= \left(\lim_{\Delta z \to 0} \Delta z\right) + 2z = 2z,$$

from which we see immediately that the limit both exists and is independent of the way in which $\Delta z \to 0$. Thus we have verified that $f(z) = z^2$ is differentiable for all (finite) z. We also note that the derivative is analogous to that found for real variables.

Although the definition of a differentiable function clearly includes a wide class of functions, the concept of differentiability is restrictive and, indeed, some functions are not differentiable at any point in the complex plane.

►*Show that the function $f(z) = 2y + ix$ is not differentiable anywhere in the complex plane.*

In this case $f(z)$ cannot be written simply in terms of z, and so we must consider the limit (24.1) in terms of x and y explicitly. Following the same procedure as in the previous example we find

$$\frac{f(z+\Delta z) - f(z)}{\Delta z} = \frac{2y + 2\Delta y + ix + i\Delta x - 2y - ix}{\Delta x + i\Delta y}$$
$$= \frac{2\Delta y + i\Delta x}{\Delta x + i\Delta y}.$$

In this case the limit will clearly depend on the direction from which $\Delta z \to 0$. Suppose $\Delta z \to 0$ along a line through z of slope m, so that $\Delta y = m\Delta x$, then

$$\lim_{\Delta z \to 0}\left[\frac{f(z+\Delta z) - f(z)}{\Delta z}\right] = \lim_{\Delta x, \Delta y \to 0}\left[\frac{2\Delta y + i\Delta x}{\Delta x + i\Delta y}\right] = \frac{2m + i}{1 + im}.$$

This limit is dependent on m and hence on the direction from which $\Delta z \to 0$. Since this conclusion is independent of the value of z, and hence true for all z, $f(z) = 2y + ix$ is nowhere differentiable. ◄

A function that is single-valued and differentiable at all points of a domain R is said to be *analytic* (or *regular*) in R. A function may be analytic in a domain except at a finite number of points (or an infinite number if the domain is infinite); in this case it is said to be analytic except at these points, which are called the *singularities* of $f(z)$. In our treatment we will not consider cases in which an infinite number of singularities occur in a finite domain.

►*Show that the function $f(z) = 1/(1-z)$ is analytic everywhere except at $z = 1$.*

Since $f(z)$ is given explicitly as a function of z, evaluation of the limit (24.1) is somewhat easier. We find

$$\begin{aligned} f'(z) &= \lim_{\Delta z \to 0} \left[\frac{f(z+\Delta z) - f(z)}{\Delta z} \right] \\ &= \lim_{\Delta z \to 0} \left[\frac{1}{\Delta z} \left(\frac{1}{1-z-\Delta z} - \frac{1}{1-z} \right) \right] \\ &= \lim_{\Delta z \to 0} \left[\frac{1}{(1-z-\Delta z)(1-z)} \right] = \frac{1}{(1-z)^2}, \end{aligned}$$

independently of the way in which $\Delta z \to 0$, provided $z \neq 1$. Hence $f(z)$ is analytic everywhere except at the singularity $z = 1$. ◄

24.2 The Cauchy–Riemann relations

From examining the previous examples, it is apparent that for a function $f(z)$ to be differentiable and hence analytic there must be some particular connection between its real and imaginary parts u and v.

By considering a general function we next establish what this connection must be. If the limit

$$L = \lim_{\Delta z \to 0} \left[\frac{f(z+\Delta z) - f(z)}{\Delta z} \right] \tag{24.2}$$

is to exist and be unique, in the way required for differentiability, then any two specific ways of letting $\Delta z \to 0$ must produce the same limit. In particular, moving parallel to the real axis and moving parallel to the imaginary axis must do so. This is certainly a necessary condition, although it may not be sufficient.

If we let $f(z) = u(x, y) + iv(x, y)$ and $\Delta z = \Delta x + i\Delta y$ then we have

$$f(z+\Delta z) = u(x+\Delta x,\ y+\Delta y) + iv(x+\Delta x,\ y+\Delta y),$$

and the limit (24.2) is given by

$$L = \lim_{\Delta x, \Delta y \to 0} \left[\frac{u(x+\Delta x, y+\Delta y) + iv(x+\Delta x, y+\Delta y) - u(x,y) - iv(x,y)}{\Delta x + i\Delta y} \right].$$

If we first suppose that Δz is purely real, so that $\Delta y = 0$, we obtain

$$L = \lim_{\Delta x \to 0} \left[\frac{u(x+\Delta x, y) - u(x,y)}{\Delta x} + i\frac{v(x+\Delta x, y) - v(x,y)}{\Delta x} \right] = \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}, \tag{24.3}$$

provided each limit exists at the point z. Similarly, if Δz is taken as purely imaginary, so that $\Delta x = 0$, we find

$$L = \lim_{\Delta y \to 0} \left[\frac{u(x, y+\Delta y) - u(x,y)}{i\Delta y} + i\frac{v(x, y+\Delta y) - v(x,y)}{i\Delta y} \right] = \frac{1}{i}\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}. \tag{24.4}$$

For f to be differentiable at the point z, expressions (24.3) and (24.4) must be identical. It follows from equating real and imaginary parts that *necessary* conditions for this are

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \qquad \text{and} \qquad \frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}. \tag{24.5}$$

These two equations are known as the *Cauchy–Riemann relations*.

We can now see why for the earlier examples (i) $f(z) = x^2 - y^2 + i2xy$ might be differentiable and (ii) $f(z) = 2y + ix$ could not be.

(i) $u = x^2 - y^2$, $v = 2xy$:

$$\frac{\partial u}{\partial x} = 2x = \frac{\partial v}{\partial y} \qquad \text{and} \qquad \frac{\partial v}{\partial x} = 2y = -\frac{\partial u}{\partial y},$$

(ii) $u = 2y$, $v = x$:

$$\frac{\partial u}{\partial x} = 0 = \frac{\partial v}{\partial y} \qquad \text{but} \qquad \frac{\partial v}{\partial x} = 1 \neq -2 = -\frac{\partial u}{\partial y}.$$

It is apparent that for $f(z)$ to be analytic something more than the existence of the partial derivatives of u and v with respect to x and y is required; this something is that they satisfy the Cauchy–Riemann relations.

We may enquire also as to the *sufficient* conditions for $f(z)$ to be analytic in R. It can be shown[§] that a sufficient condition is that the four partial derivatives exist, *are continuous* and satisfy the Cauchy–Riemann relations. It is the additional requirement of continuity that makes the difference between the necessary conditions and the sufficient conditions.

► *In which domain(s) of the complex plane is $f(z) = |x| - i|y|$ an analytic function?*

Writing $f = u + iv$ it is clear that both $\partial u/\partial y$ and $\partial v/\partial x$ are zero in all four quadrants and hence that the second Cauchy–Riemann relation in (24.5) is satisfied everywhere.

Turning to the first Cauchy–Riemann relation, in the first quadrant ($x > 0$, $y > 0$) we have $f(z) = x - iy$ so that

$$\frac{\partial u}{\partial x} = 1, \qquad \frac{\partial v}{\partial y} = -1,$$

which clearly violates the first relation in (24.5). Thus $f(z)$ is not analytic in the first quadrant.

Following a similiar argument for the other quadrants, we find

$$\frac{\partial u}{\partial x} = -1 \quad \text{or} \quad +1 \qquad \text{for } x < 0 \text{ and } x > 0, \text{ respectively,}$$
$$\frac{\partial v}{\partial y} = -1 \quad \text{or} \quad +1 \qquad \text{for } y > 0 \text{ and } y < 0, \text{ respectively.}$$

Therefore $\partial u/\partial x$ and $\partial v/\partial y$ are equal, and hence $f(z)$ is analytic only in the second and fourth quadrants. ◄

[§] See, for example, any of the references given on page 824.

Since x and y are related to z and its complex conjugate z^* by

$$x = \frac{1}{2}(z + z^*) \qquad \text{and} \qquad y = \frac{1}{2i}(z - z^*), \tag{24.6}$$

we may formally regard any function $f = u + iv$ as a function of z and z^*, rather than x and y. If we do this and examine $\partial f/\partial z^*$ we obtain

$$\begin{aligned}\frac{\partial f}{\partial z^*} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial z^*} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial z^*} \\ &= \left(\frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}\right)\left(\frac{1}{2}\right) + \left(\frac{\partial u}{\partial y} + i\frac{\partial v}{\partial y}\right)\left(-\frac{1}{2i}\right) \\ &= \frac{1}{2}\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) + \frac{i}{2}\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right).\end{aligned} \tag{24.7}$$

Now, if f is analytic then the Cauchy–Riemann relations (24.5) must be satisfied, and these immediately give that $\partial f/\partial z^*$ is identically zero. Thus we conclude that if f is analytic then f cannot be a function of z^* and any expression representing an analytic function of z can contain x and y only in the combination $x + iy$, *not* in the combination $x - iy$.

We conclude this section by discussing some properties of analytic functions that are of great practical importance in theoretical physics. These can be obtained simply from the requirement that the Cauchy–Riemann relations must be satisfied by the real and imaginary parts of an analytic function.

The most important of these results can be obtained by differentiating the first Cauchy–Riemann relation with respect to one independent variable, and the second with respect to the other independent variable, to obtain the two chains of equalities

$$\begin{aligned}\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) &= \frac{\partial}{\partial x}\left(\frac{\partial v}{\partial y}\right) = \frac{\partial}{\partial y}\left(\frac{\partial v}{\partial x}\right) = -\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial y}\right), \\ \frac{\partial}{\partial x}\left(\frac{\partial v}{\partial x}\right) &= -\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right) = -\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right) = -\frac{\partial}{\partial y}\left(\frac{\partial v}{\partial y}\right).\end{aligned}$$

Thus both u and v are *separately* solutions of Laplace's equation in two dimensions, i.e.

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \qquad \text{and} \qquad \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} = 0. \tag{24.8}$$

We will make significant use of this result in the next chapter.

A further useful result concerns the two families of curves $u(x, y) =$ constant and $v(x, y) =$ constant, where u and v are the real and imaginary parts of any analytic function $f = u + iv$. As discussed in chapter 10, the vector normal to the curve $u(x, y) =$ constant is given by

$$\nabla u = \frac{\partial u}{\partial x}\mathbf{i} + \frac{\partial u}{\partial y}\mathbf{j}, \tag{24.9}$$

where **i** and **j** are the unit vectors along the x- and y-axes, respectively. A similar expression exists for ∇v, the normal to the curve $v(x, y) =$ constant. Taking the scalar product of these two normal vectors, we obtain

$$\begin{aligned}\nabla u \cdot \nabla v &= \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial y} \\ &= -\frac{\partial u}{\partial x}\frac{\partial u}{\partial y} + \frac{\partial u}{\partial y}\frac{\partial u}{\partial x} = 0,\end{aligned}$$

where in the last line we have used the Cauchy–Riemann relations to rewrite the partial derivatives of v as partial derivatives of u. Since the scalar product of the normal vectors is zero, they must be orthogonal, and the curves $u(x, y) =$ constant and $v(x, y) =$ constant must therefore intersect at *right angles.*

► *Use the Cauchy–Riemann relations to show that, for any analytic function $f = u + iv$, the relation $|\nabla u| = |\nabla v|$ must hold.*

From (24.9) we have

$$|\nabla u|^2 = \nabla u \cdot \nabla u = \left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2.$$

Using the Cauchy–Riemann relations to write the partial derivatives of u in terms of those of v, we obtain

$$|\nabla u|^2 = \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial v}{\partial x}\right)^2 = |\nabla v|^2,$$

from which the result $|\nabla u| = |\nabla v|$ follows immediately. ◄

24.3 Power series in a complex variable

The theory of power series in a real variable was considered in chapter 4, which also contained a brief discussion of the natural extension of this theory to a series such as

$$f(z) = \sum_{n=0}^{\infty} a_n z^n, \tag{24.10}$$

where z is a complex variable and the a_n are, in general, complex. We now consider complex power series in more detail.

Expression (24.10) is a power series about the origin and may be used for general discussion, since a power series about any other point z_0 can be obtained by a change of variable from z to $z - z_0$. If z were written in its modulus and argument form, $z = r \exp i\theta$, expression (24.10) would become

$$f(z) = \sum_{n=0}^{\infty} a_n r^n \exp(in\theta). \tag{24.11}$$

This series is absolutely convergent if

$$\sum_{n=0}^{\infty} |a_n| r^n, \tag{24.12}$$

which is a series of positive real terms, is convergent. Thus tests for the absolute convergence of real series can be used in the present context, and of these the most appropriate form is based on the Cauchy root test. With the *radius of convergence* R defined by

$$\frac{1}{R} = \lim_{n\to\infty} |a_n|^{1/n}, \tag{24.13}$$

the series (24.10) is absolutely convergent if $|z| < R$ and divergent if $|z| > R$. If $|z| = R$ then no particular conclusion may be drawn, and this case must be considered separately, as discussed in subsection 4.5.1.

A circle of radius R centred on the origin is called the *circle of convergence* of the series $\sum a_n z^n$. The cases $R = 0$ and $R = \infty$ correspond, respectively, to convergence at the origin only and convergence everywhere. For R finite the convergence occurs in a restricted part of the z-plane (the Argand diagram). For a power series about a general point z_0, the circle of convergence is, of course, centred on that point.

►*Find the parts of the z-plane for which the following series are convergent:*

$$\text{(i)} \sum_{n=0}^{\infty} \frac{z^n}{n!}, \qquad \text{(ii)} \sum_{n=0}^{\infty} n! z^n, \qquad \text{(iii)} \sum_{n=1}^{\infty} \frac{z^n}{n}.$$

(i) Since $(n!)^{1/n}$ behaves like n as $n \to \infty$ we find $\lim(1/n!)^{1/n} = 0$. Hence $R = \infty$ and the series is convergent for all z. (ii) Correspondingly, $\lim(n!)^{1/n} = \infty$. Thus $R = 0$ and the series converges only at $z = 0$. (iii) As $n \to \infty$, $(n)^{1/n}$ has a lower limit of 1 and hence $\lim(1/n)^{1/n} = 1/1 = 1$. Thus the series is absolutely convergent if the condition $|z| < 1$ is satisfied. ◄

Case (iii) in the above example provides a good illustration of the fact that on its circle of convergence a power series may or may not converge. For this particular series, the circle of convergence is $|z| = 1$, so let us consider the convergence of the series at two different points on this circle. Taking $z = 1$, the series becomes

$$\sum_{n=1}^{\infty} \frac{1}{n} = 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \cdots,$$

which is easily shown to diverge (by, for example, grouping terms, as discussed in subsection 4.3.2). Taking $z = -1$, however, the series is given by

$$\sum_{n=1}^{\infty} \frac{(-1)^n}{n} = -1 + \frac{1}{2} - \frac{1}{3} + \frac{1}{4} - \cdots,$$

which is an alternating series whose terms decrease in magnitude and which therefore converges.

The ratio test discussed in subsection 4.3.2 may also be employed to investigate the absolute convergence of a complex power series. A series is absolutely convergent if

$$\lim_{n\to\infty} \frac{|a_{n+1}||z|^{n+1}}{|a_n||z|^n} = \lim_{n\to\infty} \frac{|a_{n+1}||z|}{|a_n|} < 1 \tag{24.14}$$

and hence the radius of convergence R of the series is given by

$$\frac{1}{R} = \lim_{n\to\infty} \frac{|a_{n+1}|}{|a_n|}.$$

For instance, in case (i) of the previous example, we have

$$\frac{1}{R} = \lim_{n\to\infty} \frac{n!}{(n+1)!} = \lim_{n\to\infty} \frac{1}{n+1} = 0.$$

Thus the series is absolutely convergent for all (finite) z, confirming the previous result.

Before turning to particular power series, we conclude this section by stating the important result[§] that *the power series* $\sum_0^\infty a_n z^n$ *has a sum that is an analytic function of* z *inside its circle of convergence*.

As a corollary to the above theorem, it may further be shown that if $f(z) = \sum a_n z^n$ then, inside the circle of convergence of the series,

$$f'(z) = \sum_{n=0}^{\infty} n a_n z^{n-1}.$$

Repeated application of this result demonstrates that any power series can be differentiated any number of times inside its circle of convergence.

24.4 Some elementary functions

In the example at the end of the previous section it was shown that the function $\exp z$ *defined* by

$$\exp z = \sum_{n=0}^{\infty} \frac{z^n}{n!} \tag{24.15}$$

is convergent for all z of finite modulus and is thus, by the discussion of the previous section, an analytic function over the whole z-plane.[¶] Like its

[§] For a proof see, for example, K. F. Riley, *Mathematical Methods for the Physical Sciences* (Cambridge: Cambridge University Press, 1974), p. 446.

[¶] Functions that are analytic in the *whole* z-plane are usually called *integral* or *entire* functions.

real-variable counterpart it is called the *exponential function*; also like its real counterpart it is equal to its own derivative.

The multiplication of two exponential functions results in a further exponential function, in accordance with the corresponding result for real variables.

►*Show that* $\exp z_1 \exp z_2 = \exp(z_1 + z_2)$.

From the series expansion (24.15) of $\exp z_1$ and a similar expansion for $\exp z_2$, it is clear that the coefficient of $z_1^r z_2^s$ in the corresponding series expansion of $\exp z_1 \exp z_2$ is simply $1/(r!s!)$.

But, from (24.15) we also have

$$\exp(z_1 + z_2) = \sum_{n=0}^{\infty} \frac{(z_1 + z_2)^n}{n!}.$$

In order to find the coefficient of $z_1^r z_2^s$ in this expansion, we clearly have to consider the term in which $n = r + s$, namely

$$\frac{(z_1 + z_2)^{r+s}}{(r+s)!} = \frac{1}{(r+s)!}\left({}^{r+s}C_0 z_1^{r+s} + \cdots + {}^{r+s}C_s z_1^r z_2^s + \cdots + {}^{r+s}C_{r+s} z_2^{r+s}\right).$$

The coefficient of $z_1^r z_2^s$ in this is given by

$${}^{r+s}C_s \frac{1}{(r+s)!} = \frac{(r+s)!}{s!r!}\frac{1}{(r+s)!} = \frac{1}{r!s!}.$$

Thus, since the corresponding coefficients on the two sides are equal, and all the series involved are absolutely convergent for all z, we can conclude that $\exp z_1 \exp z_2 = \exp(z_1 + z_2)$. ◄

As an extension of (24.15) we may also define the complex exponent of a real number $a > 0$ by the equation

$$a^z = \exp(z \ln a), \tag{24.16}$$

where $\ln a$ is the natural logarithm of a. The particular case $a = e$ and the fact that $\ln e = 1$ enable us to write $\exp z$ interchangeably with e^z. If z is real then the definition agrees with the familiar one.

The result for $z = iy$,

$$\exp iy = \cos y + i \sin y, \tag{24.17}$$

has been met already in equation (3.23). Its immediate extension is

$$\exp z = (\exp x)(\cos y + i \sin y). \tag{24.18}$$

As z varies over the complex plane, the modulus of $\exp z$ takes all real positive values, except that of 0. However, two values of z that differ by $2\pi ki$, for any integer k, produce the same value of $\exp z$, as given by (24.18), and so $\exp z$ is periodic with period $2\pi i$. If we denote $\exp z$ by t, then the strip $-\pi < y \leq \pi$ in the z-plane corresponds to the whole of the t-plane, except for the point $t = 0$.

The sine, cosine, sinh and cosh functions of a complex variable are defined from the exponential function exactly as are those for real variables. The functions

derived from them (e.g. tan and tanh), the identities they satisfy and their derivative properties are also just as for real variables. In view of this we will not give them further attention here.

The inverse function of $\exp z$ is given by w, the solution of

$$\exp w = z. \tag{24.19}$$

This inverse function was discussed in chapter 3, but we mention it again here for completeness. By virtue of the discussion following (24.18), w is not uniquely defined and is indeterminate to the extent of any integer multiple of $2\pi i$. If we express z as

$$z = r \exp i\theta,$$

where r is the (real) modulus of z and θ is its argument ($-\pi < \theta \leq \pi$), then multiplying z by $\exp(2ik\pi)$, where k is an integer, will result in the same complex number z. Thus we may write

$$z = r \exp[i(\theta + 2k\pi)],$$

where k is an integer. If we denote w in (24.19) by

$$w = \operatorname{Ln} z = \ln r + i(\theta + 2k\pi), \tag{24.20}$$

where $\ln r$ is the natural logarithm (to base e) of the real positive quantity r, then $\operatorname{Ln} z$ is an infinitely multivalued function of z. Its *principal value*, denoted by $\ln z$, is obtained by taking $k = 0$ so that its argument lies in the range $-\pi$ to π. Thus

$$\ln z = \ln r + i\theta, \qquad \text{with } -\pi < \theta \leq \pi. \tag{24.21}$$

Now that the logarithm of a complex variable has been defined, definition (24.16) of a general power can be extended to cases other than those in which a is real and positive. If t ($\neq 0$) and z are both complex, then the zth power of t is defined by

$$t^z = \exp(z \operatorname{Ln} t). \tag{24.22}$$

Since $\operatorname{Ln} t$ is multivalued, so is this definition. Its principal value is obtained by giving $\operatorname{Ln} t$ its principal value, $\ln t$.

If t ($\neq 0$) is complex but z is real and equal to $1/n$, then (24.22) provides a definition of the nth root of t. Because of the multivaluedness of $\operatorname{Ln} t$, there will be more than one nth root of any given t.

►*Show that there are exactly n distinct nth roots of t.*

From (24.22) the nth roots of t are given by

$$t^{1/n} = \exp\left(\frac{1}{n} \operatorname{Ln} t\right).$$

On the RHS let us write t as follows:

$$t = r\exp[i(\theta + 2k\pi)],$$

where k is an integer. We then obtain

$$t^{1/n} = \exp\left[\frac{1}{n}\ln r + i\frac{(\theta + 2k\pi)}{n}\right]$$
$$= r^{1/n}\exp\left[i\frac{(\theta + 2k\pi)}{n}\right],$$

where $k = 0, 1, \ldots, n-1$; for other values of k we simply recover the roots already found. Thus t has n distinct nth roots. ◄

24.5 Multivalued functions and branch cuts

In the definition of an analytic function, one of the conditions imposed was that the function is single-valued. However, as shown in the previous section, the logarithmic function, a complex power and a complex root are all multivalued. Nevertheless, it happens that the properties of analytic functions can still be applied to these and other multivalued functions of a complex variable provided that suitable care is taken. This care amounts to identifying the *branch points* of the multivalued function $f(z)$ in question. If z is varied in such a way that its path in the Argand diagram forms a closed curve that encloses a branch point, then, in general, $f(z)$ will not return to its original value.

For definiteness let us consider the multivalued function $f(z) = z^{1/2}$ and express z as $z = r\exp i\theta$. From figure 24.1(a), it is clear that, as the point z traverses any closed contour C that does not enclose the origin, θ will return to its original value after one complete circuit. However, for any closed contour C' that does enclose the origin, after one circuit $\theta \to \theta + 2\pi$ (see figure 24.1(b)). Thus, for the function $f(z) = z^{1/2}$, after one circuit

$$r^{1/2}\exp(i\theta/2) \;\to\; r^{1/2}\exp[i(\theta + 2\pi)/2] = -r^{1/2}\exp(i\theta/2).$$

In other words, the value of $f(z)$ changes around any closed loop enclosing the origin; in this case $f(z) \to -f(z)$. Thus $z = 0$ is a branch point of the function $f(z) = z^{1/2}$.

We note in this case that if any closed contour enclosing the origin is traversed *twice* then $f(z) = z^{1/2}$ returns to its original value. The number of loops around a branch point required for any given function $f(z)$ to return to its original value depends on the function in question, and for some functions (e.g. $\mathrm{Ln}\, z$, which also has a branch point at the origin) the original value is never recovered.

In order that $f(z)$ may be treated as single-valued, we may define a *branch cut* in the Argand diagram. A branch cut is a line (or curve) in the complex plane and may be regarded as an artificial barrier that we must not cross. Branch cuts are positioned in such a way that we are prevented from making a complete

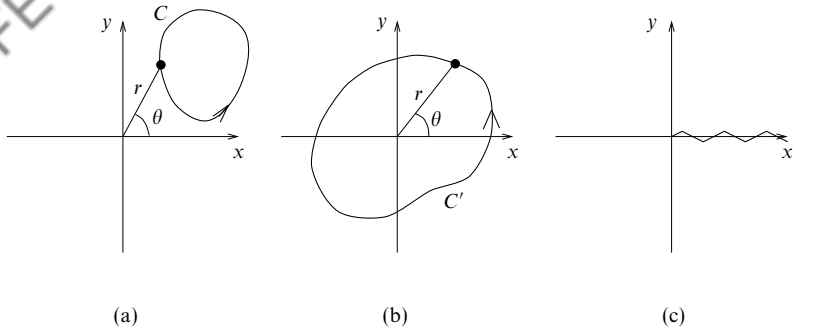


Figure 24.1 (a) A closed contour not enclosing the origin; (b) a closed contour enclosing the origin; (c) a possible branch cut for $f(z) = z^{1/2}$.

circuit around any one branch point, and so the function in question remains single-valued.

For the function $f(z) = z^{1/2}$, we may take as a branch cut any curve starting at the origin $z = 0$ and extending out to $|z| = \infty$ in any direction, since all such curves would equally well prevent us from making a closed loop around the branch point at the origin. It is usual, however, to take the cut along either the real or the imaginary axis. For example, in figure 24.1(c), we take the cut as the positive real axis. By agreeing not to cross this cut, we restrict θ to lie in the range $0 \leq \theta < 2\pi$, and so keep $f(z)$ single-valued.

These ideas are easily extended to functions with more than one branch point.

► *Find the branch points of* $f(z) = \sqrt{z^2 + 1}$, *and hence sketch suitable arrangements of branch cuts.*

We begin by writing $f(z)$ as

$$f(z) = \sqrt{z^2 + 1} = \sqrt{(z - i)(z + i)}.$$

As shown above, the function $g(z) = z^{1/2}$ has a branch point at $z = 0$. Thus we might expect $f(z)$ to have branch points at values of z that make the expression under the square root equal to zero, i.e. at $z = i$ and $z = -i$.

As shown in figure 24.2(a), we use the notation

$$z - i = r_1 \exp i\theta_1 \qquad \text{and} \qquad z + i = r_2 \exp i\theta_2.$$

We can therefore write $f(z)$ as

$$f(z) = \sqrt{r_1 r_2}\exp(i\theta_1/2)\exp(i\theta_2/2) = \sqrt{r_1 r_2}\exp\left[i(\theta_1 + \theta_2)/2\right].$$

Let us now consider how $f(z)$ changes as we make one complete circuit around various closed loops C in the Argand diagram. If C encloses

(i) neither branch point, then $\theta_1 \to \theta_1$, $\theta_2 \to \theta_2$ and so $f(z) \to f(z)$;
(ii) $z = i$ but not $z = -i$, then $\theta_1 \to \theta_1 + 2\pi$, $\theta_2 \to \theta_2$ and so $f(z) \to -f(z)$;

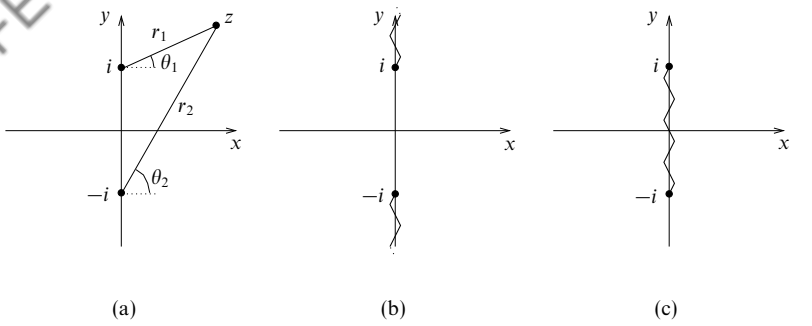


Figure 24.2 (a) Coordinates used in the analysis of the branch points of $f(z) = (z^2 + 1)^{1/2}$; (b) one possible arrangement of branch cuts; (c) another possible branch cut, which is finite.

(iii) $z = -i$ but not $z = i$, then $\theta_1 \to \theta_1$, $\theta_2 \to \theta_2 + 2\pi$ and so $f(z) \to -f(z)$;
(iv) both branch points, then $\theta_1 \to \theta_1 + 2\pi$, $\theta_2 \to \theta_2 + 2\pi$ and so $f(z) \to f(z)$.

Thus, as expected, $f(z)$ changes value around loops containing either $z = i$ or $z = -i$ (but not both). We must therefore choose branch cuts that prevent us from making a complete loop around either branch point; one suitable choice is shown in figure 24.2(b).

For this $f(z)$, however, we have noted that after traversing a loop containing *both* branch points the function returns to its original value. Thus we may choose an alternative, *finite*, branch cut that allows this possibility but still prevents us from making a complete loop around just one of the points. A suitable cut is shown in figure 24.2(c). ◄

24.6 Singularities and zeros of complex functions

A singular point of a complex function $f(z)$ is any point in the Argand diagram at which $f(z)$ fails to be analytic. We have already met one sort of singularity, the branch point, and in this section we will consider other types of singularity as well as discuss the zeros of complex functions.

If $f(z)$ has a singular point at $z = z_0$ but is analytic at all points in some neighbourhood containing z_0 but no other singularities, then $z = z_0$ is called an *isolated singularity*. (Clearly, branch points are not isolated singularities.)

The most important type of isolated singularity is the *pole*. If $f(z)$ has the form

$$f(z) = \frac{g(z)}{(z - z_0)^n}, \tag{24.23}$$

where n is a positive integer, $g(z)$ is analytic at all points in some neighbourhood containing $z = z_0$ and $g(z_0) \neq 0$, then $f(z)$ has a *pole of order n* at $z = z_0$. An alternative (though equivalent) definition is that

$$\lim_{z \to z_0} [(z - z_0)^n f(z)] = a, \tag{24.24}$$

where a is a finite, non-zero complex number. We note that if the above limit is equal to zero, then $z = z_0$ is a pole of order less than n, or $f(z)$ is analytic there; if the limit is infinite then the pole is of an order greater than n. It may also be shown that if $f(z)$ has a pole at $z = z_0$, then $|f(z)| \to \infty$ as $z \to z_0$ from any direction in the Argand diagram.[§] If no finite value of n can be found such that (24.24) is satisfied, then $z = z_0$ is called an *essential singularity*.

► *Find the singularities of the functions*

$$\text{(i) } f(z) = \frac{1}{1-z} - \frac{1}{1+z}, \qquad \text{(ii) } f(z) = \tanh z.$$

(i) If we write $f(z)$ as

$$f(z) = \frac{1}{1-z} - \frac{1}{1+z} = \frac{2z}{(1-z)(1+z)},$$

we see immediately from either (24.23) or (24.24) that $f(z)$ has poles of order 1 (or *simple poles*) at $z = 1$ and $z = -1$.

(ii) In this case we write

$$f(z) = \tanh z = \frac{\sinh z}{\cosh z} = \frac{\exp z - \exp(-z)}{\exp z + \exp(-z)}.$$

Thus $f(z)$ has a singularity when $\exp z = -\exp(-z)$ or, equivalently, when

$$\exp z = \exp[i(2n+1)\pi]\exp(-z),$$

where n is any integer. Equating the arguments of the exponentials we find $z = (n + \frac{1}{2})\pi i$, for integer n.

Furthermore, using l'Hôpital's rule (see chapter 4) we have

$$\lim_{z\to(n+\frac{1}{2})\pi i}\left\{\frac{[z-(n+\tfrac{1}{2})\pi i]\sinh z}{\cosh z}\right\} = \lim_{z\to(n+\frac{1}{2})\pi i}\left\{\frac{[z-(n+\tfrac{1}{2})\pi i]\cosh z + \sinh z}{\sinh z}\right\} = 1.$$

Therefore, from (24.24), each singularity is a simple pole. ◄

Another type of singularity exists at points for which the value of $f(z)$ takes an indeterminate form such as $0/0$ but $\lim_{z\to z_0} f(z)$ exists and is independent of the direction from which z_0 is approached. Such points are called *removable singularities*.

► *Show that* $f(z) = (\sin z)/z$ *has a removable singularity at* $z = 0$.

It is clear that $f(z)$ takes the indeterminate form $0/0$ at $z = 0$. However, by expanding $\sin z$ as a power series in z, we find

$$f(z) = \frac{1}{z}\left(z - \frac{z^3}{3!} + \frac{z^5}{5!} - \cdots\right) = 1 - \frac{z^2}{3!} + \frac{z^4}{5!} - \cdots.$$

[§] Although perhaps intuitively obvious, this result really requires formal demonstration by analysis.

Thus $\lim_{z\to 0} f(z) = 1$ independently of the way in which $z \to 0$, and so $f(z)$ has a removable singularity at $z = 0$. ◄

An expression common in mathematics, but which we have so far avoided using explicitly in this chapter, is 'z tends to infinity'. For a real variable such as $|z|$ or R, 'tending to infinity' has a reasonably well defined meaning. For a complex variable needing a two-dimensional plane to represent it, the meaning is not intrinsically well defined. However, it is convenient to have a unique meaning and this is provided by the following *definition*: the behaviour of $f(z)$ *at infinity* is given by that of $f(1/\xi)$ at $\xi = 0$, where $\xi = 1/z$.

►*Find the behaviour at infinity of* (i) $f(z) = a + bz^{-2}$, (ii) $f(z) = z(1 + z^2)$ *and* (iii) $f(z) = \exp z$.

(i) $f(z) = a + bz^{-2}$: on putting $z = 1/\xi$, $f(1/\xi) = a + b\xi^2$, which is analytic at $\xi = 0$; thus f is analytic at $z = \infty$.
(ii) $f(z) = z(1 + z^2)$: $f(1/\xi) = 1/\xi + 1/\xi^3$; thus f has a pole of order 3 at $z = \infty$.
(iii) $f(z) = \exp z$: $f(1/\xi) = \sum_0^\infty (n!)^{-1}\xi^{-n}$; thus f has an essential singularity at $z = \infty$. ◄

We conclude this section by briefly mentioning the *zeros* of a complex function. As the name suggests, if $f(z_0) = 0$ then $z = z_0$ is called a zero of the function $f(z)$. Zeros are classified in a similar way to poles, in that if

$$f(z) = (z - z_0)^n g(z),$$

where n is a positive integer and $g(z_0) \neq 0$, then $z = z_0$ is called a *zero of order* n of $f(z)$. If $n = 1$ then $z = z_0$ is called a *simple zero*. It may further be shown that if $z = z_0$ is a zero of order n of $f(z)$ then it is also a pole of order n of the function $1/f(z)$.

We will return in section 24.11 to the classification of zeros and poles in terms of their series expansions.

24.7 Conformal transformations

We now turn our attention to the subject of transformations, by which we mean a change of coordinates from the complex variable $z = x + iy$ to another, say $w = r + is$, by means of a prescribed formula:

$$w = g(z) = r(x, y) + is(x, y).$$

Under such a transformation, or *mapping*, the Argand diagram for the z-variable is transformed into one for the w-variable, although the complete z-plane might be mapped onto only a part of the w-plane, or onto the whole of the w-plane, or onto some or all of the w-plane covered more than once.

We shall consider only those mappings for which w and z are related by a function $w = g(z)$ and its inverse $z = h(w)$ with both functions analytic, except possibly at a few isolated points; such mappings are called *conformal*. Their

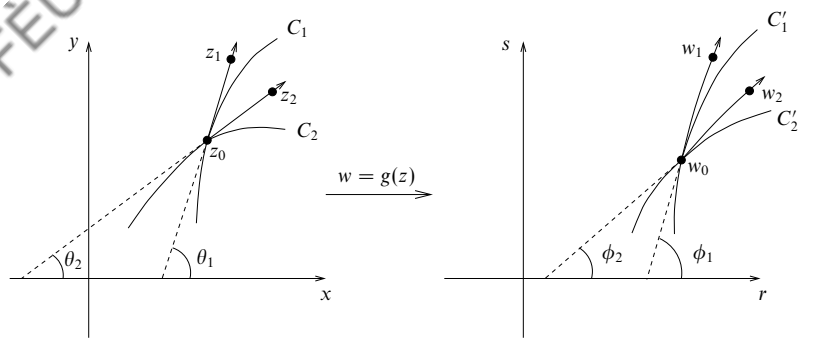


Figure 24.3 Two curves C_1 and C_2 in the z-plane, which are mapped onto C_1' and C_2' in the w-plane.

important properties are that, except at points at which $g'(z)$, and hence $h'(z)$, is zero or infinite:

(i) continuous lines in the z-plane transform into continuous lines in the w-plane;
(ii) the angle between two intersecting curves in the z-plane equals the angle between the corresponding curves in the w-plane;
(iii) the magnification, as between the z-plane and the w-plane, of a small line element in the neighbourhood of any particular point is independent of the direction of the element;
(iv) any analytic function of z transforms to an analytic function of w and vice versa.

Result (i) is immediate, and results (ii) and (iii) can be justified by the following argument. Let two curves C_1 and C_2 pass through the point z_0 in the z-plane and let z_1 and z_2 be two points on their respective tangents at z_0, each a distance ρ from z_0. The same prescription with w replacing z describes the transformed situation; however, the transformed tangents may not be straight lines and the distances of w_1 and w_2 from w_0 have not yet been shown to be equal. This situation is illustrated in figure 24.3.

In the z-plane z_1 and z_2 are given by

$$z_1 - z_0 = \rho \exp i\theta_1 \qquad \text{and} \qquad z_2 - z_0 = \rho \exp i\theta_2.$$

The corresponding descriptions in the w-plane are

$$w_1 - w_0 = \rho_1 \exp i\phi_1 \qquad \text{and} \qquad w_2 - w_0 = \rho_2 \exp i\phi_2.$$

The angles θ_i and ϕ_i are clear from figure 24.3. The transformed angles ϕ_i are those made with the r-axis by the tangents to the transformed curves at their

point of intersection. Since any finite-length tangent may be curved, w_i is more strictly given by $w_i - w_0 = \rho_i \exp i(\phi_i + \delta\phi_i)$, where $\delta\phi_i \to 0$ as $\rho_i \to 0$, i.e. as $\rho \to 0$.

Now since $w = g(z)$, where g is analytic, we have

$$\lim_{z_1 \to z_0} \left(\frac{w_1 - w_0}{z_1 - z_0} \right) = \lim_{z_2 \to z_0} \left(\frac{w_2 - w_0}{z_2 - z_0} \right) = \left. \frac{dg}{dz} \right|_{z=z_0},$$

which may be written as

$$\lim_{\rho \to 0} \left\{ \frac{\rho_1}{\rho} \exp[i(\phi_1 + \delta\phi_1 - \theta_1)] \right\} = \lim_{\rho \to 0} \left\{ \frac{\rho_2}{\rho} \exp[i(\phi_2 + \delta\phi_2 - \theta_2)] \right\} = g'(z_0). \tag{24.25}$$

Comparing magnitudes and phases (i.e. arguments) in the equalities (24.25) gives the stated results (ii) and (iii) and adds quantitative information to them, namely that for *small* line elements

$$\frac{\rho_1}{\rho} \approx \frac{\rho_2}{\rho} \approx |g'(z_0)|, \tag{24.26}$$

$$\phi_1 - \theta_1 \approx \phi_2 - \theta_2 \approx \arg g'(z_0). \tag{24.27}$$

For strict comparison with result (ii), (24.27) must be written as $\theta_1 - \theta_2 = \phi_1 - \phi_2$, with an ordinary equality sign, since the angles are only defined in the limit $\rho \to 0$ when (24.27) becomes a true identity. We also see from (24.26) that the linear magnification factor is $|g'(z_0)|$; similarly, small areas are magnified by $|g'(z_0)|^2$.

Since in the neighbourhoods of corresponding points in a transformation angles are preserved and magnifications are independent of direction, it follows that small plane figures are transformed into figures of the same shape, but, in general, ones that are magnified and rotated (though not distorted). However, we also note that at points where $g'(z) = 0$, the angle $\arg g'(z)$ through which line elements are rotated is undefined; these are called *critical points* of the transformation.

The final result (iv) is perhaps the most important property of conformal transformations. If $f(z)$ is an analytic function of z and $z = h(w)$ is also analytic, then $F(w) = f(h(w))$ is analytic in w. Its importance lies in the further conclusions it allows us to draw from the fact that, since f is analytic, the real and imaginary parts of $f = \phi + i\psi$ are necessarily solutions of

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \qquad \text{and} \qquad \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = 0. \tag{24.28}$$

Since the transformation property ensures that $F = \Phi + i\Psi$ is also analytic, we can conclude that its real and imaginary parts must themselves satisfy Laplace's equation in the w-plane:

$$\frac{\partial^2 \Phi}{\partial r^2} + \frac{\partial^2 \Phi}{\partial s^2} = 0 \qquad \text{and} \qquad \frac{\partial^2 \Psi}{\partial r^2} + \frac{\partial^2 \Psi}{\partial s^2} = 0. \tag{24.29}$$

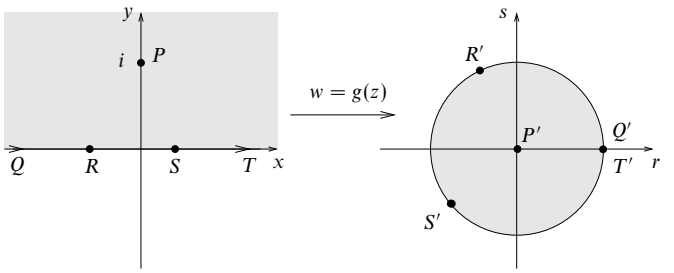


Figure 24.4 Transforming the upper half of the z-plane into the interior of the unit circle in the w-plane, in such a way that $z = i$ is mapped onto $w = 0$ and the points $x = \pm\infty$ are mapped onto $w = 1$.

Further, suppose that (say) Re $f(z) = \phi$ is constant over a boundary C in the z-plane; then Re $F(w) = \Phi$ is constant over C in the z-plane. But this is the same as saying that Re $F(w)$ is constant over the boundary C' in the w-plane, C' being the curve into which C is transformed by the conformal transformation $w = g(z)$. This result is exploited extensively in the next chapter to solve Laplace's equation for a variety of two-dimensional geometries.

Examples of useful conformal transformations are numerous. For instance, $w = z + b$, $w = (\exp i\phi)z$ and $w = az$ correspond, respectively, to a translation by b, a rotation through an angle ϕ and a stretching (or contraction) in the radial direction (for a real). These three examples can be combined into the general linear transformation $w = az + b$, where, in general, a and b are complex. Another example is the inversion mapping $w = 1/z$, which maps the interior of the unit circle to the exterior and vice versa. Other, more complicated, examples also exist.

►*Show that if the point z_0 lies in the upper half of the z-plane then the transformation*

$$w = (\exp i\phi)\frac{z - z_0}{z - z_0^*}$$

maps the upper half of the z-plane into the interior of the unit circle in the w-plane. Hence find a similar transformation that maps the point $z = i$ onto $w = 0$ and the points $x = \pm\infty$ onto $w = 1$.

Taking the modulus of w, we have

$$|w| = \left|(\exp i\phi)\frac{z - z_0}{z - z_0^*}\right| = \left|\frac{z - z_0}{z - z_0^*}\right|.$$

However, since the complex conjugate z_0^* is the reflection of z_0 in the real axis, if z and z_0 both lie in the upper half of the z-plane then $|z - z_0| \leq |z - z_0^*|$; thus $|w| \leq 1$, as required. We also note that (i) the equality holds only when z lies on the real axis, and so this axis is mapped onto the boundary of the unit circle in the w-plane; (ii) the point z_0 is mapped onto $w = 0$, the origin of the w-plane.

By fixing the images of two points in the z-plane, the constants z_0 and ϕ can also be fixed. Since we require the point $z = i$ to be mapped onto $w = 0$, we have immediately

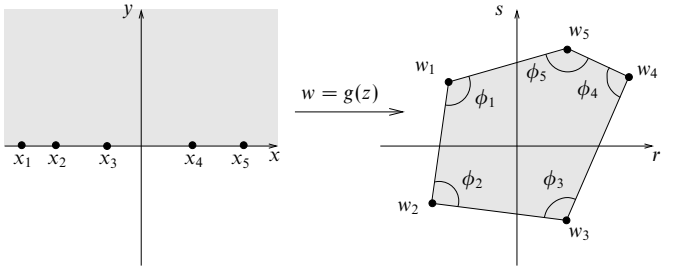


Figure 24.5 Transforming the upper half of the z-plane into the interior of a polygon in the w-plane, in such a way that the points $x_1, x_2, \ldots, x_n$ are mapped onto the vertices $w_1, w_2, \ldots, w_n$ of the polygon with interior angles $\phi_1, \phi_2, \ldots, \phi_n$.

$z_0 = i$. By further requiring $z = \pm\infty$ to be mapped onto $w = 1$, we find $1 = w = \exp i\phi$ and so $\phi = 0$. The required transformation is therefore

$$w = \frac{z - i}{z + i},$$

and is illustrated in figure 24.4. ◄

We conclude this section by mentioning the rather curious *Schwarz–Christoffel* transformation.§ Suppose, as shown in figure 24.5, that we are interested in a (finite) number of points $x_1, x_2, \ldots, x_n$ on the real axis in the z-plane. Then by means of the transformation

$$w = \left\{ A \int_0^z (\xi - x_1)^{(\phi_1/\pi)-1} (\xi - x_2)^{(\phi_2/\pi)-1} \cdots (\xi - x_n)^{(\phi_n/\pi)-1} \, d\xi \right\} + B, \quad (24.30)$$

we may map the upper half of the z-plane onto the interior of a closed polygon in the w-plane having n vertices $w_1, w_2, \ldots, w_n$ (which are the images of $x_1, x_2, \ldots, x_n$) with corresponding interior angles $\phi_1, \phi_2, \ldots, \phi_n$, as shown in figure 24.5. The real axis in the z-plane is transformed into the boundary of the polygon itself. The constants A and B are complex in general and determine the position, size and orientation of the polygon. It is clear from (24.30) that $dw/dz = 0$ at $x = x_1, x_2, \ldots, x_n$, and so the transformation is not conformal at these points.

There are various subtleties associated with the use of the Schwarz–Christoffel transformation. For example, if one of the points on the real axis in the z-plane (usually x_n) is taken at infinity, then the corresponding factor in (24.30) (i.e. the one involving x_n) is not present. In this case, the point(s) $x = \pm\infty$ are considered as one point, since they transform to a single vertex of the polygon in the w-plane.

§ Strictly speaking, the use of this transformation requires an understanding of complex integrals, which are discussed in section 24.8.

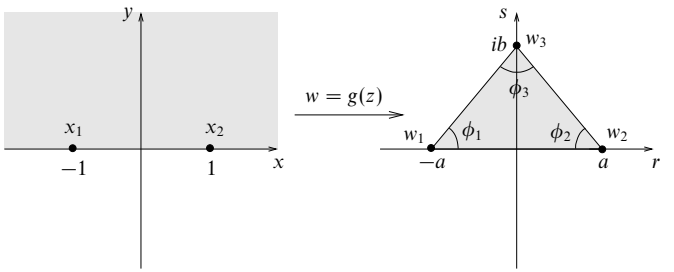


Figure 24.6 Transforming the upper half of the z-plane into the interior of a triangle in the w-plane.

We can also map the upper half of the z-plane into an infinite *open* polygon by considering it as the limiting case of some closed polygon.

► *Find a transformation that maps the upper half of the z-plane into the triangular region shown in figure 24.6 in such a way that the points* $x_1 = -1$ *and* $x_2 = 1$ *are mapped into the points* $w = -a$ *and* $w = a$*, respectively, and the point* $x_3 = \pm\infty$ *is mapped into* $w = ib$*. Hence find a transformation that maps the upper half of the z-plane into the region* $-a < r < a$*,* $s > 0$ *of the w-plane, as shown in figure 24.7.*

Let us denote the angles at w_1 and w_2 in the w-plane by $\phi_1 = \phi_2 = \phi$, where $\phi = \tan^{-1}(b/a)$. Since x_3 is taken at infinity, we may omit the corresponding factor in (24.30) to obtain

$$\begin{aligned} w &= \left\{ A \int_0^z (\xi + 1)^{(\phi/\pi)-1} (\xi - 1)^{(\phi/\pi)-1}\, d\xi \right\} + B \\ &= \left\{ A \int_0^z (\xi^2 - 1)^{(\phi/\pi)-1}\, d\xi \right\} + B. \end{aligned} \tag{24.31}$$

The required transformation may then be found by fixing the constants A and B as follows. Since the point $z = 0$ lies on the line segment x_1x_2, it will be mapped onto the line segment w_1w_2 in the w-plane, and by symmetry must be mapped onto the point $w = 0$. Thus setting $z = 0$ and $w = 0$ in (24.31) we obtain $B = 0$. An expression for A can be found in the form of an integral by setting (for example) $z = 1$ and $w = a$ in (24.31).

We may consider the region in the w-plane in figure 24.7 to be the limiting case of the triangular region in figure 24.6 with the vertex w_3 at infinity. Thus we may use the above, but with the angles at w_1 and w_2 set to $\phi = \pi/2$. From (24.31), we obtain

$$w = A \int_0^z \frac{d\xi}{\sqrt{\xi^2 - 1}} = iA \sin^{-1} z.$$

By setting $z = 1$ and $w = a$, we find $iA = 2a/\pi$, so the required transformation is

$$w = \frac{2a}{\pi} \sin^{-1} z. \blacktriangleleft$$

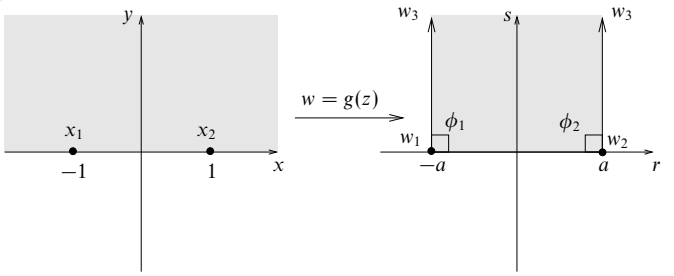


Figure 24.7 Transforming the upper half of the z-plane into the interior of the region $-a < r < a$, $s > 0$ in the w-plane.

24.8 Complex integrals

Corresponding to integration with respect to a real variable, it is possible to define integration with respect to a complex variable between two complex limits. Since the z-plane is two-dimensional there is clearly greater freedom and hence ambiguity in what is meant by a complex integral. If a complex function $f(z)$ is single-valued and continuous in some region R in the complex plane, then we can define the complex integral of $f(z)$ between two points A and B along some curve in R; its value will depend, in general, upon the path taken between A and B (see figure 24.8). However, we will find that for some paths that are different but bear a particular relationship to each other the value of the integral does *not* depend upon which of the paths is adopted.

Let a particular path C be described by a continuous (real) parameter t ($\alpha \leq t \leq \beta$) that gives successive positions on C by means of the equations

$$x = x(t), \qquad y = y(t), \tag{24.32}$$

with $t = \alpha$ and $t = \beta$ corresponding to the points A and B, respectively. Then the integral along path C of a continuous function $f(z)$ is written

$$\int_C f(z)\, dz \tag{24.33}$$

and can be given explicitly as a sum of real integrals as follows:

$$\begin{aligned}\int_C f(z)\, dz &= \int_C (u + iv)(dx + i dy) \\ &= \int_C u\, dx - \int_C v\, dy + i \int_C u\, dy + i \int_C v\, dx \\ &= \int_\alpha^\beta u \frac{dx}{dt}\, dt - \int_\alpha^\beta v \frac{dy}{dt}\, dt + i \int_\alpha^\beta u \frac{dy}{dt}\, dt + i \int_\alpha^\beta v \frac{dx}{dt}\, dt.\end{aligned} \tag{24.34}$$

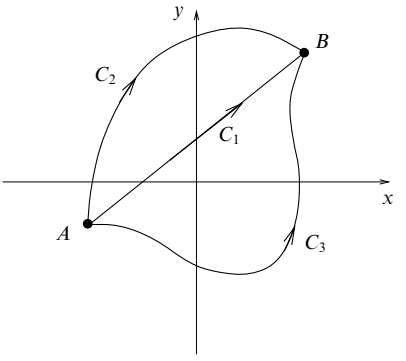


Figure 24.8 Some alternative paths for the integral of a function $f(z)$ between A and B.

The question of when such an integral exists will not be pursued, except to state that a sufficient condition is that dx/dt and dy/dt are continuous.

► *Evaluate the complex integral of $f(z) = z^{-1}$ along the circle $|z| = R$, starting and finishing at $z = R$.*

The path C_1 is parameterised as follows (figure 24.9(a)):

$$z(t) = R\cos t + iR\sin t, \qquad 0 \leq t \leq 2\pi,$$

whilst $f(z)$ is given by

$$f(z) = \frac{1}{x+iy} = \frac{x-iy}{x^2+y^2}.$$

Thus the real and imaginary parts of $f(z)$ are

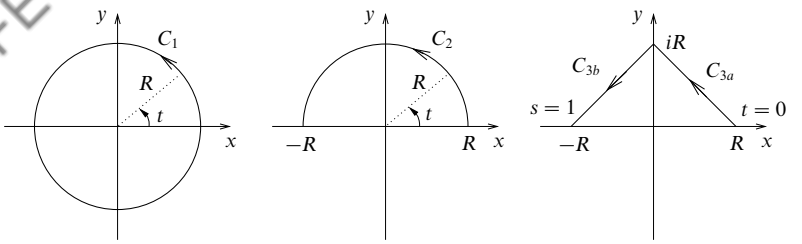
$$u = \frac{x}{x^2+y^2} = \frac{R\cos t}{R^2} \qquad \text{and} \qquad v = \frac{-y}{x^2+y^2} = -\frac{R\sin t}{R^2}.$$

Hence, using expression (24.34),

$$\begin{aligned}\int_{C_1} \frac{1}{z}\,dz &= \int_0^{2\pi} \frac{\cos t}{R}(-R\sin t)\,dt - \int_0^{2\pi} \left(\frac{-\sin t}{R}\right) R\cos t\,dt \\ &\quad + i\int_0^{2\pi} \frac{\cos t}{R} R\cos t\,dt + i\int_0^{2\pi} \left(\frac{-\sin t}{R}\right)(-R\sin t)\,dt \qquad (24.35) \\ &= 0 + 0 + i\pi + i\pi = 2\pi i. \blacktriangleleft\end{aligned}$$

With a bit of experience, the reader may be able to evaluate integrals like the LHS of (24.35) directly without having to write them as four separate real integrals. In the present case,

$$\int_{C_1} \frac{dz}{z} = \int_0^{2\pi} \frac{-R\sin t + iR\cos t}{R\cos t + iR\sin t}\,dt = \int_0^{2\pi} i\,dt = 2\pi i. \qquad (24.36)$$



(a) (b) (c)

Figure 24.9 Different paths for an integral of $f(z) = z^{-1}$. See the text for details.

This very important result will be used many times later, and the following should be carefully noted: (i) its value, (ii) that this value is independent of R.

In the above example the contour was closed, and so it began and ended at the same point in the Argand diagram. We can evaluate complex integrals along open paths in a similar way.

► *Evaluate the complex integral of* $f(z) = z^{-1}$ *along the following paths (see figure 24.9):*
(i) *the contour* C_2 *consisting of the semicircle* $|z| = R$ *in the half-plane* $y \geq 0$,
(ii) *the contour* C_3 *made up of the two straight lines* C_{3a} *and* C_{3b}.

(i) This is just as in the previous example, except that now $0 \leq t \leq \pi$. With this change, we have from (24.35) or (24.36) that

$$\int_{C_2} \frac{dz}{z} = \pi i. \tag{24.37}$$

(ii) The straight lines that make up the countour C_3 may be parameterised as follows:

$$\begin{aligned} &C_{3a}, \qquad z = (1-t)R + itR \qquad \text{for } 0 \leq t \leq 1; \\ &C_{3b}, \qquad z = -sR + i(1-s)R \qquad \text{for } 0 \leq s \leq 1. \end{aligned}$$

With these parameterisations the required integrals may be written

$$\int_{C_3} \frac{dz}{z} = \int_0^1 \frac{-R+iR}{R+t(-R+iR)}\,dt + \int_0^1 \frac{-R-iR}{iR+s(-R-iR)}\,ds. \tag{24.38}$$

If we could take over from real-variable theory that, for real t, $\int (a+bt)^{-1}\,dt = b^{-1}\ln(a+bt)$ even if a and b are complex, then these integrals could be evaluated immediately. However, to do this would be presuming to some extent what we wish to show, and so the evaluation

must be made in terms of entirely real integrals. For example, the first is given by

$$\begin{aligned}\int_0^1 \frac{-R+iR}{R(1-t)+itR}\,dt &= \int_0^1 \frac{(-1+i)(1-t-it)}{(1-t)^2+t^2}\,dt \\ &= \int_0^1 \frac{2t-1}{1-2t+2t^2}\,dt + i\int_0^1 \frac{1}{1-2t+2t^2}\,dt \\ &= \frac{1}{2}\left[\ln(1-2t+2t^2)\right]_0^1 + \frac{i}{2}\left[2\tan^{-1}\left(\frac{t-\frac{1}{2}}{\frac{1}{2}}\right)\right]_0^1 \\ &= 0 + \frac{i}{2}\left[\frac{\pi}{2} - \left(-\frac{\pi}{2}\right)\right] = \frac{\pi i}{2}.\end{aligned}$$

The second integral on the RHS of (24.38) can also be shown to have the value $\pi i/2$. Thus

$$\int_{C_3} \frac{dz}{z} = \pi i. \blacktriangleleft$$

Considering the results of the preceding two examples, which have common integrands and limits, some interesting observations are possible. Firstly, the two integrals from $z = R$ to $z = -R$, along C_2 and C_3, respectively, have the same value, even though the paths taken are different. It also follows that if we took a closed path C_4, given by C_2 from R to $-R$ and C_3 traversed backwards from $-R$ to R, then the integral round C_4 of z^{-1} would be zero (both parts contributing equal and opposite amounts). This is to be compared with result (24.36), in which closed path C_1, beginning and ending at the same place as C_4, yields a value $2\pi i$.

It is not true, however, that the integrals along the paths C_2 and C_3 are equal for any function $f(z)$, or, indeed, that their values are independent of R in general.

►*Evaluate the complex integral of* $f(z) = \mathrm{Re}\, z$ *along the paths* C_1, C_2 *and* C_3 *shown in figure 24.9.*

(i) If we take $f(z) = \mathrm{Re}\, z$ and the contour C_1 then

$$\int_{C_1} \mathrm{Re}\, z\; dz = \int_0^{2\pi} R\cos t(-R\sin t + iR\cos t)\; dt = i\pi R^2.$$

(ii) Using C_2 as the contour,

$$\int_{C_2} \mathrm{Re}\, z\; dz = \int_0^{\pi} R\cos t(-R\sin t + iR\cos t)\; dt = \tfrac{1}{2}i\pi R^2.$$

(iii) Finally the integral along $C_3 = C_{3a} + C_{3b}$ is given by

$$\begin{aligned}\int_{C_3} \mathrm{Re}\, z\; dz &= \int_0^1 (1-t)R(-R+iR)\; dt + \int_0^1 (-sR)(-R-iR)\; ds \\ &= \tfrac{1}{2}R^2(-1+i) + \tfrac{1}{2}R^2(1+i) = iR^2. \blacktriangleleft\end{aligned}$$

The results of this section demonstrate that the value of an integral between the same two points may depend upon the path that is taken between them but, at the same time, suggest that, under some circumstances, the value is independent of the path. The general situation is summarised in the result of the next section,

namely Cauchy's theorem, which is the cornerstone of the integral calculus of complex variables.

Before discussing Cauchy's theorem, however, we note an important result concerning complex integrals that will be of some use later. Let us consider the integral of a function $f(z)$ along some path C. If M is an upper bound on the value of $|f(z)|$ on the path, i.e. $|f(z)| \leq M$ on C, and L is the length of the path C, then

$$\left| \int_C f(z)\, dz \right| \leq \int_c |f(z)||dz| \leq M \int_C dl = ML. \tag{24.39}$$

It is straightforward to verify that this result does indeed hold for the complex integrals considered earlier in this section.

24.9 Cauchy's theorem

Cauchy's theorem states that if $f(z)$ is an analytic function, and $f'(z)$ is continuous at each point within and on a closed contour C, then

$$\oint_C f(z)\, dz = 0. \tag{24.40}$$

In this statement and from now on we denote an integral around a closed contour by $\oint_C$.

To prove this theorem we will need the two-dimensional form of the divergence theorem, known as Green's theorem in a plane (see section 11.3). This says that if p and q are two functions with continuous first derivatives within and on a closed contour C (bounding a domain R) in the xy-plane, then

$$\iint_R \left(\frac{\partial p}{\partial x} + \frac{\partial q}{\partial y} \right) dx dy = \oint_C (p\, dy - q\, dx). \tag{24.41}$$

With $f(z) = u + iv$ and $dz = dx + i\, dy$, this can be applied to

$$I = \oint_C f(z)\, dz = \oint_C (u\, dx - v\, dy) + i \oint_C (v\, dx + u\, dy)$$

to give

$$I = \iint_R \left[\frac{\partial(-u)}{\partial y} + \frac{\partial(-v)}{\partial x} \right] dx\, dy + i \iint_R \left[\frac{\partial(-v)}{\partial y} + \frac{\partial u}{\partial x} \right] dx\, dy. \tag{24.42}$$

Now, recalling that $f(z)$ is analytic and therefore that the Cauchy–Riemann relations (24.5) apply, we see that each integrand is identically zero and thus I is also zero; this proves Cauchy's theorem.

In fact, the conditions of the above proof are more stringent than they need be. The continuity of $f'(z)$ is not necessary for the proof of Cauchy's theorem,

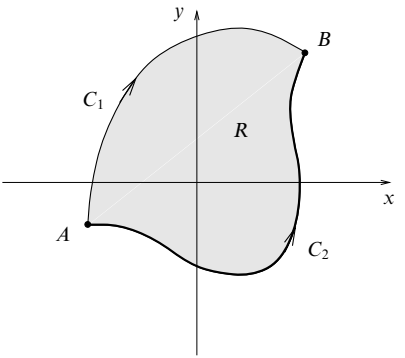


Figure 24.10 Two paths C_1 and C_2 enclosing a region R.

analyticity of $f(z)$ within and on C being sufficient. However, the proof then becomes more complicated and is too long to be given here.[§]

The connection between Cauchy's theorem and the zero value of the integral of z^{-1} around the composite path C_4 discussed towards the end of the previous section is apparent: the function z^{-1} is analytic in the two regions of the z-plane enclosed by contours (C_2 and C_{3a}) and (C_2 and C_{3b}).

►*Suppose two points A and B in the complex plane are joined by two different paths C_1 and C_2. Show that if $f(z)$ is an analytic function on each path and in the region enclosed by the two paths, then the integral of $f(z)$ is the same along C_1 and C_2.*

The situation is shown in figure 24.10. Since $f(z)$ is analytic in R, it follows from Cauchy's theorem that we have

$$\int_{C_1} f(z)\,dz - \int_{C_2} f(z)\,dz = \oint_{C_1 - C_2} f(z)\,dz = 0,$$

since $C_1 - C_2$ forms a closed contour enclosing R. Thus we immediately obtain

$$\int_{C_1} f(z)\,dz = \int_{C_2} f(z)\,dz,$$

and so the values of the integrals along C_1 and C_2 are equal. ◄

An important application of Cauchy's theorem is in proving that, in some cases, it is possible to deform a closed contour C into another contour γ in such a way that the integrals of a function $f(z)$ around each of the contours have the same value.

[§] The reader may refer to almost any book that is devoted to complex variables and the theory of functions.

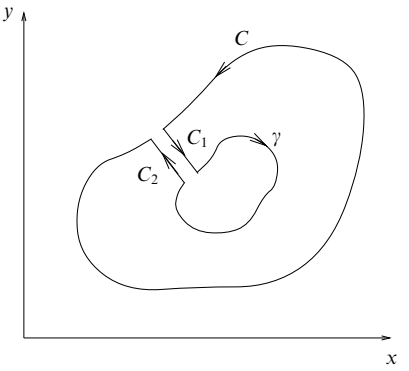


Figure 24.11 The contour used to prove the result (24.43).

►*Consider two closed contours C and γ in the Argand diagram, γ being sufficiently small that it lies completely within C. Show that if the function $f(z)$ is analytic in the region between the two contours then*

$$\oint_C f(z)\,dz = \oint_\gamma f(z)\,dz. \tag{24.43}$$

To prove this result we consider a contour as shown in figure 24.11. The two close parallel lines C_1 and C_2 join γ and C, which are 'cut' to accommodate them. The new contour Γ so formed consists of C, C_1, γ and C_2.

Within the area bounded by Γ, the function $f(z)$ is analytic, and therefore, by Cauchy's theorem (24.40),

$$\oint_\Gamma f(z)\,dz = 0. \tag{24.44}$$

Now the parts C_1 and C_2 of Γ are traversed in opposite directions, and in the limit lie on top of each other, and so their contributions to (24.44) cancel. Thus

$$\oint_C f(z)\,dz + \oint_\gamma f(z)\,dz = 0. \tag{24.45}$$

The sense of the integral round γ is opposite to the conventional (anticlockwise) one, and so by traversing γ in the usual sense, we establish the result (24.43). ◄

A sort of converse of Cauchy's theorem is known as *Morera's theorem*, which states that if $f(z)$ is a continuous function of z in a closed domain R bounded by a curve C and, further, $\oint_C f(z)\,dz = 0$, then $f(z)$ is analytic in R.

24.10 Cauchy's integral formula

Another very important theorem in the theory of complex variables is *Cauchy's integral formula*, which states that if $f(z)$ is analytic within and on a closed

contour C and z_0 is a point within C then

$$f(z_0) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{z - z_0}\, dz. \tag{24.46}$$

This formula is saying that the value of an analytic function anywhere inside a closed contour is uniquely determined by its values on the contour[§] and that the specific expression (24.46) can be given for the value at the interior point.

We may prove Cauchy's integral formula by using (24.43) and taking γ to be a circle centred on the point $z = z_0$, of small enough radius ρ that it all lies inside C. Then, since $f(z)$ is analytic inside C, the integrand $f(z)/(z - z_0)$ is analytic in the space between C and γ. Thus, from (24.43), the integral around γ has the same value as that around C.

We then use the fact that any point z on γ is given by $z = z_0 + \rho \exp i\theta$ (and so $dz = i\rho \exp i\theta\ d\theta$). Thus the value of the integral around γ is given by

$$\begin{aligned} I = \oint_\gamma \frac{f(z)}{z - z_0}\, dz &= \int_0^{2\pi} \frac{f(z_0 + \rho \exp i\theta)}{\rho \exp i\theta} i\rho \exp i\theta\ d\theta \\ &= i\int_0^{2\pi} f(z_0 + \rho \exp i\theta)\ d\theta. \end{aligned}$$

If the radius of the circle γ is now shrunk to zero, i.e. $\rho \to 0$, then $I \to 2\pi i f(z_0)$, thus establishing the result (24.46).

An extension to Cauchy's integral formula can be made, yielding an integral expression for $f'(z_0)$:

$$f'(z_0) = \frac{1}{2\pi i}\int_C \frac{f(z)}{(z - z_0)^2}\, dz, \tag{24.47}$$

under the same conditions as previously stated.

►*Prove Cauchy's integral formula for $f'(z_0)$ given in (24.47).*

To show this, we use the definition of a derivative and (24.46) itself to evaluate

$$\begin{aligned} f'(z_0) &= \lim_{h\to 0} \frac{f(z_0 + h) - f(z_0)}{h} \\ &= \lim_{h\to 0} \left[\frac{1}{2\pi i}\oint_C \frac{f(z)}{h}\left(\frac{1}{z - z_0 - h} - \frac{1}{z - z_0}\right) dz\right] \\ &= \lim_{h\to 0} \left[\frac{1}{2\pi i}\oint_C \frac{f(z)}{(z - z_0 - h)(z - z_0)}\, dz\right] \\ &= \frac{1}{2\pi i}\oint_C \frac{f(z)}{(z - z_0)^2}\, dz, \end{aligned}$$

which establishes result (24.47). ◄

[§] The similarity between this and the uniqueness theorem for the Laplace equation with Dirichlet boundary conditions (see chapter 20) is apparent.

Further, it may be proved by induction that the nth derivative of $f(z)$ is also given by a Cauchy integral,

$$f^{(n)}(z_0) = \frac{n!}{2\pi i}\oint_C \frac{f(z)\,dz}{(z-z_0)^{n+1}}. \tag{24.48}$$

Thus, if the value of the analytic function is known on C then not only may the value of the function at any interior point be calculated, but also the values of *all* its derivatives.

The observant reader will notice that (24.48) may also be obtained by the formal device of differentiating under the integral sign with respect to z_0 in Cauchy's integral formula (24.46):

$$\begin{aligned} f^{(n)}(z_0) &= \frac{1}{2\pi i}\oint_C \frac{\partial^n}{\partial z_0^n}\left[\frac{f(z)}{(z-z_0)}\right] dz \\ &= \frac{n!}{2\pi i}\oint_C \frac{f(z)\,dz}{(z-z_0)^{n+1}}. \end{aligned}$$

►*Suppose that $f(z)$ is analytic inside and on a circle C of radius R centred on the point $z = z_0$. If $|f(z)| \le M$ on the circle, where M is some constant, show that*

$$|f^{(n)}(z_0)| \le \frac{Mn!}{R^n}. \tag{24.49}$$

From (24.48) we have

$$|f^{(n)}(z_0)| = \frac{n!}{2\pi}\left|\oint_C \frac{f(z)\,dz}{(z-z_0)^{n+1}}\right|,$$

and on using (24.39) this becomes

$$|f^{(n)}(z_0)| \le \frac{n!}{2\pi}\frac{M}{R^{n+1}}2\pi R = \frac{Mn!}{R^n}.$$

This result is known as *Cauchy's inequality*. ◄

We may use Cauchy's inequality to prove *Liouville's theorem*, which states that if $f(z)$ is analytic and bounded for all z then f is a constant. Setting $n = 1$ in (24.49) and letting $R \to \infty$, we find $|f'(z_0)| = 0$ and hence $f'(z_0) = 0$. Since $f(z)$ is analytic for all z, we may take z_0 as any point in the z-plane and thus $f'(z) = 0$ for all z; this implies $f(z) =$ constant. Liouville's theorem may be used in turn to prove the *fundamental theorem of algebra* (see exercise 24.9).

24.11 Taylor and Laurent series

Following on from (24.48), we may establish *Taylor's theorem* for functions of a complex variable. If $f(z)$ is analytic inside and on a circle C of radius R centred on the point $z = z_0$, and z is a point inside C, then

$$f(z) = \sum_{n=0}^{\infty} a_n(z-z_0)^n, \tag{24.50}$$

where a_n is given by $f^{(n)}(z_0)/n!$. The Taylor expansion is valid inside the region of analyticity and, for any particular z_0, can be shown to be unique.

To prove Taylor's theorem (24.50), we note that, since $f(z)$ is analytic inside and on C, we may use Cauchy's formula to write $f(z)$ as

$$f(z) = \frac{1}{2\pi i}\oint_C \frac{f(\xi)}{\xi - z}\, d\xi, \tag{24.51}$$

where ξ lies on C. Now we may expand the factor $(\xi - z)^{-1}$ as a geometric series in $(z - z_0)/(\xi - z_0)$,

$$\frac{1}{\xi - z} = \frac{1}{\xi - z_0}\sum_{n=0}^{\infty}\left(\frac{z - z_0}{\xi - z_0}\right)^n,$$

so (24.51) becomes

$$\begin{aligned} f(z) &= \frac{1}{2\pi i}\oint_C \frac{f(\xi)}{\xi - z_0}\sum_{n=0}^{\infty}\left(\frac{z - z_0}{\xi - z_0}\right)^n d\xi \\ &= \frac{1}{2\pi i}\sum_{n=0}^{\infty}(z - z_0)^n \oint_C \frac{f(\xi)}{(\xi - z_0)^{n+1}}\, d\xi \\ &= \frac{1}{2\pi i}\sum_{n=0}^{\infty}(z - z_0)^n \frac{2\pi i f^{(n)}(z_0)}{n!}, \end{aligned} \tag{24.52}$$

where we have used Cauchy's integral formula (24.48) for the derivatives of $f(z)$. Cancelling the factors of $2\pi i$, we thus establish the result (24.50) with $a_n = f^{(n)}(z_0)/n!$.

►*Show that if $f(z)$ and $g(z)$ are analytic in some region R, and $f(z) = g(z)$ within some subregion S of R, then $f(z) = g(z)$ throughout R.*

It is simpler to consider the (analytic) function $h(z) = f(z) - g(z)$, and to show that because $h(z) = 0$ in S it follows that $h(z) = 0$ throughout R.

If we choose a point $z = z_0$ in S, then we can expand $h(z)$ in a Taylor series about z_0,

$$h(z) = h(z_0) + h'(z_0)(z - z_0) + \tfrac{1}{2}h''(z_0)(z - z_0)^2 + \cdots,$$

which will converge inside some circle C that extends at least as far as the nearest part of the boundary of R, since $h(z)$ is analytic in R. But since z_0 lies in S, we have

$$h(z_0) = h'(z_0) = h''(z_0) = \cdots = 0,$$

and so $h(z) = 0$ inside C. We may now expand about a new point, which can lie anywhere within C, and repeat the process. By continuing this procedure we may show that $h(z) = 0$ throughout R.

This result is called the *identity theorem* and, in fact, the equality of $f(z)$ and $g(z)$ throughout R follows from their equality along any curve of non-zero length in R, or even at a countably infinite number of points in R. ◄

So far we have assumed that $f(z)$ is analytic inside and on the (circular) contour C. If, however, $f(z)$ has a singularity inside C at the point $z = z_0$, then it cannot be expanded in a Taylor series. Nevertheless, suppose that $f(z)$ has a pole

of order p at $z = z_0$ but is analytic at every other point inside and on C. Then the function $g(z) = (z - z_0)^p f(z)$ is analytic at $z = z_0$, and so may be expanded as a Taylor series about $z = z_0$:

$$g(z) = \sum_{n=0}^{\infty} b_n (z - z_0)^n. \tag{24.53}$$

Thus, for all z inside C, $f(z)$ will have a power series representation of the form

$$f(z) = \frac{a_{-p}}{(z - z_0)^p} + \cdots + \frac{a_{-1}}{z - z_0} + a_0 + a_1(z - z_0) + a_2(z - z_0)^2 + \cdots, \tag{24.54}$$

with $a_{-p} \neq 0$. Such a series, which is an extension of the Taylor expansion, is called a *Laurent series*. By comparing the coefficients in (24.53) and (24.54), we see that $a_n = b_{n+p}$. Now, the coefficients b_n in the Taylor expansion of $g(z)$ are seen from (24.52) to be given by

$$b_n = \frac{g^{(n)}(z_0)}{n!} = \frac{1}{2\pi i} \oint \frac{g(z)}{(z - z_0)^{n+1}}\, dz,$$

and so for the coefficients a_n in (24.54) we have

$$a_n = \frac{1}{2\pi i} \oint \frac{g(z)}{(z - z_0)^{n+1+p}}\, dz = \frac{1}{2\pi i} \oint \frac{f(z)}{(z - z_0)^{n+1}}\, dz,$$

an expression that is valid for both positive and negative n.

The terms in the Laurent series with $n \geq 0$ are collectively called the *analytic part*, whilst the remainder of the series, consisting of terms in inverse powers of $z - z_0$, is called the *principal part*. Depending on the nature of the point $z = z_0$, the principal part may contain an infinite number of terms, so that

$$f(z) = \sum_{n=-\infty}^{+\infty} a_n (z - z_0)^n. \tag{24.55}$$

In this case we would expect the principal part to converge only for $|(z - z_0)^{-1}|$ less than some constant, i.e. *outside* some circle centred on z_0. However, the analytic part will converge *inside* some (different) circle also centred on z_0. If the latter circle has the greater radius then the Laurent series will converge in the region R *between* the two circles (see figure 24.12); otherwise it does not converge at all.

In fact, it may be shown that any function $f(z)$ that is analytic in a region R between two such circles C_1 and C_2 centred on $z = z_0$ can be expressed as a Laurent series about z_0 that converges in R. We note that, depending on the nature of the point $z = z_0$, the inner circle may be a point (when the principal part contains only a finite number of terms) and the outer circle may have an infinite radius.

We may use the Laurent series of a function $f(z)$ about any point $z = z_0$ to

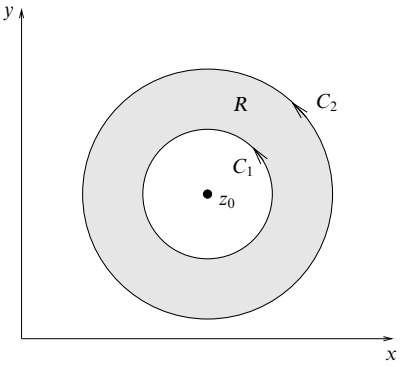


Figure 24.12 The region of convergence R for a Laurent series of $f(z)$ about a point $z = z_0$ where $f(z)$ has a singularity.

classify the nature of that point. If $f(z)$ is actually analytic at $z = z_0$, then in (24.55) all a_n for $n < 0$ must be zero. It may happen that not only are all a_n zero for $n < 0$ but $a_0, a_1, \ldots, a_{m-1}$ are all zero as well. In this case, the first non-vanishing term in (24.55) is $a_m(z - z_0)^m$, with $m > 0$, and $f(z)$ is then said to have a *zero of order m* at $z = z_0$.

If $f(z)$ is not analytic at $z = z_0$, then two cases arise, as discussed above (p is here taken as positive):

(i) it is possible to find an integer p such that $a_{-p} \neq 0$ but $a_{-p-k} = 0$ for all integers $k > 0$;

(ii) it is not possible to find such a lowest value of $-p$.

In case (i), $f(z)$ is of the form (24.54) and is described as having a *pole of order* p at $z = z_0$; the value of a_{-1} (not a_{-p}) is called the *residue* of $f(z)$ at the pole $z = z_0$, and will play an important part in later applications.

For case (ii), in which the negatively decreasing powers of $z - z_0$ do not terminate, $f(z)$ is said to have an *essential singularity*. These definitions should be compared with those given in section 24.6.

►*Find the Laurent series of*

$$f(z) = \frac{1}{z(z-2)^3}$$

about the singularities $z = 0$ and $z = 2$ (separately). Hence verify that $z = 0$ is a pole of order 1 and $z = 2$ is a pole of order 3, and find the residue of $f(z)$ at each pole.

To obtain the Laurent series about $z = 0$, we make the factor in parentheses in the

denominator take the form $(1-\alpha z)$, where α is some constant, and thus obtain

$$\begin{aligned} f(z) &= -\frac{1}{8z(1-z/2)^3} \\ &= -\frac{1}{8z}\left[1+(-3)\left(-\frac{z}{2}\right)+\frac{(-3)(-4)}{2!}\left(-\frac{z}{2}\right)^2+\frac{(-3)(-4)(-5)}{3!}\left(-\frac{z}{2}\right)^3+\cdots\right] \\ &= -\frac{1}{8z}-\frac{3}{16}-\frac{3z}{16}-\frac{5z^2}{32}-\cdots . \end{aligned}$$

Since the lowest power of z is -1, the point $z=0$ is a pole of order 1. The residue of $f(z)$ at $z=0$ is simply the coefficient of z^{-1} in the Laurent expansion about that point and is equal to $-1/8$.

The Laurent series about $z=2$ is most easily found by letting $z=2+\xi$ (or $z-2=\xi$) and substituting into the expression for $f(z)$ to obtain

$$\begin{aligned} f(z) &= \frac{1}{(2+\xi)\xi^3} = \frac{1}{2\xi^3(1+\xi/2)} \\ &= \frac{1}{2\xi^3}\left[1-\left(\frac{\xi}{2}\right)+\left(\frac{\xi}{2}\right)^2-\left(\frac{\xi}{2}\right)^3+\left(\frac{\xi}{2}\right)^4-\cdots\right] \\ &= \frac{1}{2\xi^3}-\frac{1}{4\xi^2}+\frac{1}{8\xi}-\frac{1}{16}+\frac{\xi}{32}-\cdots \\ &= \frac{1}{2(z-2)^3}-\frac{1}{4(z-2)^2}+\frac{1}{8(z-2)}-\frac{1}{16}+\frac{z-2}{32}-\cdots . \end{aligned}$$

From this series we see that $z=2$ is a pole of order 3 and that the residue of $f(z)$ at $z=2$ is $1/8$. ◄

As we shall see in the next few sections, finding the residue of a function at a singularity is of crucial importance in the evaluation of complex integrals. Specifically, formulae exist for calculating the residue of a function at a particular (singular) point $z=z_0$ without having to expand the function explicitly as a Laurent series about z_0 and identify the coefficient of $(z-z_0)^{-1}$. The type of formula generally depends on the nature of the singularity at which the residue is required.

►*Suppose that $f(z)$ has a pole of order m at the point $z=z_0$. By considering the Laurent series of $f(z)$ about z_0, derive a general expression for the residue $R(z_0)$ of $f(z)$ at $z=z_0$. Hence evaluate the residue of the function*

$$f(z)=\frac{\exp iz}{(z^2+1)^2}$$

at the point $z=i$.

If $f(z)$ has a pole of order m at $z=z_0$, then its Laurent series about this point has the form

$$f(z)=\frac{a_{-m}}{(z-z_0)^m}+\cdots+\frac{a_{-1}}{(z-z_0)}+a_0+a_1(z-z_0)+a_2(z-z_0)^2+\cdots ,$$

which, on multiplying both sides of the equation by $(z-z_0)^m$, gives

$$(z-z_0)^m f(z)=a_{-m}+a_{-m+1}(z-z_0)+\cdots+a_{-1}(z-z_0)^{m-1}+\cdots .$$

Differentiating both sides $m-1$ times, we obtain

$$\frac{d^{m-1}}{dz^{m-1}}[(z-z_0)^m f(z)] = (m-1)!\, a_{-1} + \sum_{n=1}^{\infty} b_n (z-z_0)^n,$$

for some coefficients b_n. In the limit $z \to z_0$, however, the terms in the sum disappear, and after rearranging we obtain the formula

$$R(z_0) = a_{-1} = \lim_{z\to z_0} \left\{ \frac{1}{(m-1)!} \frac{d^{m-1}}{dz^{m-1}}[(z-z_0)^m f(z)] \right\}, \tag{24.56}$$

which gives the value of the residue of $f(z)$ at the point $z = z_0$.

If we now consider the function

$$f(z) = \frac{\exp iz}{(z^2+1)^2} = \frac{\exp iz}{(z+i)^2(z-i)^2},$$

we see immediately that it has poles of order 2 (*double* poles) at $z = i$ and $z = -i$. To calculate the residue at (for example) $z = i$, we may apply the formula (24.56) with $m = 2$. Performing the required differentiation, we obtain

$$\begin{aligned}\frac{d}{dz}[(z-i)^2 f(z)] &= \frac{d}{dz}\left[\frac{\exp iz}{(z+i)^2}\right] \\ &= \frac{1}{(z+i)^4}[(z+i)^2 i \exp iz - 2(\exp iz)(z+i)].\end{aligned}$$

Setting $z = i$, we find the residue is given by

$$R(i) = \frac{1}{1!}\frac{1}{16}\left(-4ie^{-1} - 4ie^{-1}\right) = -\frac{i}{2e}. \blacktriangleleft$$

An important special case of (24.56) occurs when $f(z)$ has a *simple pole* (a pole of order 1) at $z = z_0$. Then the residue at z_0 is given by

$$R(z_0) = \lim_{z\to z_0} [(z-z_0) f(z)]\,. \tag{24.57}$$

If $f(z)$ has a simple pole at $z = z_0$ and, as is often the case, has the form $g(z)/h(z)$, where $g(z)$ is analytic and non-zero at z_0 and $h(z_0) = 0$, then (24.57) becomes

$$\begin{aligned}R(z_0) &= \lim_{z\to z_0} \frac{(z-z_0)g(z)}{h(z)} = g(z_0) \lim_{z\to z_0} \frac{(z-z_0)}{h(z)} \\ &= g(z_0) \lim_{z\to z_0} \frac{1}{h'(z)} = \frac{g(z_0)}{h'(z_0)},\end{aligned} \tag{24.58}$$

where we have used l'Hôpital's rule. This result often provides the simplest way of determining the residue at a simple pole.

24.12 Residue theorem

Having seen from Cauchy's theorem that the value of an integral round a closed contour C is zero if the integrand is analytic inside the contour, it is natural to ask what value it takes when the integrand is not analytic inside C. The answer to this is contained in the residue theorem, which we now discuss.

Suppose the function $f(z)$ has a pole of order m at the point $z = z_0$, and so can be written as a Laurent series about z_0 of the form

$$f(z) = \sum_{n=-m}^{\infty} a_n (z - z_0)^n. \tag{24.59}$$

Now consider the integral I of $f(z)$ around a closed contour C that encloses $z = z_0$, but no other singular points. Using Cauchy's theorem, this integral has the same value as the integral around a circle γ of radius ρ centred on $z = z_0$, since $f(z)$ is analytic in the region between C and γ. On the circle we have $z = z_0 + \rho \exp i\theta$ (and $dz = i\rho \exp i\theta \; d\theta$), and so

$$\begin{aligned} I &= \oint_\gamma f(z) \; dz \\ &= \sum_{n=-m}^{\infty} a_n \oint (z - z_0)^n \; dz \\ &= \sum_{n=-m}^{\infty} a_n \int_0^{2\pi} i\rho^{n+1} \exp[i(n+1)\theta] \; d\theta. \end{aligned}$$

For every term in the series with $n \neq -1$, we have

$$\int_0^{2\pi} i\rho^{n+1} \exp[i(n+1)\theta] \; d\theta = \left[\frac{i\rho^{n+1} \exp[i(n+1)\theta]}{i(n+1)} \right]_0^{2\pi} = 0,$$

but for the $n = -1$ term we obtain

$$\int_0^{2\pi} i \; d\theta = 2\pi i.$$

Therefore only the term in $(z - z_0)^{-1}$ contributes to the value of the integral around γ (and therefore C), and I takes the value

$$I = \oint_C f(z) \; dz = 2\pi i a_{-1}. \tag{24.60}$$

Thus the integral around any closed contour containing a single pole of general order m (or, by extension, an essential singularity) is equal to $2\pi i$ times the residue of $f(z)$ at $z = z_0$.

If we extend the above argument to the case where $f(z)$ is continuous within and on a closed contour C and analytic, except for a finite number of poles, within C, then we arrive at the *residue theorem*

$$\oint_C f(z) \; dz = 2\pi i \sum_j R_j, \tag{24.61}$$

where $\sum_j R_j$ is the sum of the residues of $f(z)$ at its poles within C.

The method of proof is indicated by figure 24.13, in which (*a*) shows the original contour C referred to in (24.61) and (*b*) shows a contour C' giving the same value

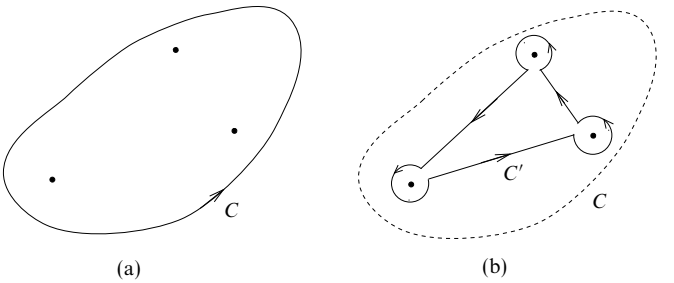


Figure 24.13 The contours used to prove the residue theorem: (a) the original contour; (b) the contracted contour encircling each of the poles.

to the integral, because f is analytic between C and C'. Now the contribution to the C' integral from the polygon (a triangle for the case illustrated) joining the small circles is zero, since f is also analytic inside C'. Hence the whole value of the integral comes from the circles and, by result (24.60), each of these contributes $2\pi i$ times the residue at the pole it encloses. All the circles are traversed in their positive sense if C is thus traversed and so the residue theorem follows. Formally, Cauchy's theorem (24.40) is a particular case of (24.61) in which C encloses no poles.

Finally we prove another important result, for later use. Suppose that $f(z)$ has a simple pole at $z = z_0$ and so may be expanded as the Laurent series

$$f(z) = \phi(z) + a_{-1}(z - z_0)^{-1},$$

where $\phi(z)$ is analytic within some neighbourhood surrounding z_0. We wish to find an expression for the integral I of $f(z)$ along an *open* contour C, which is the arc of a circle of radius ρ centred on $z = z_0$ given by

$$|z - z_0| = \rho, \qquad \theta_1 \leq \arg(z - z_0) \leq \theta_2, \tag{24.62}$$

where ρ is chosen small enough that no singularity of f, other than $z = z_0$, lies within the circle. Then I is given by

$$I = \int_C f(z)\, dz = \int_C \phi(z)\, dz + a_{-1} \int_C (z - z_0)^{-1}\, dz.$$

If the radius of the arc C is now allowed to tend to zero, then the first integral tends to zero, since the path becomes of zero length and ϕ is analytic and therefore continuous along it. On C, $z = \rho e^{i\theta}$ and hence the required expression for I is

$$I = \lim_{\rho \to 0} \int_C f(z)\, dz = \lim_{\rho \to 0} \left(a_{-1} \int_{\theta_1}^{\theta_2} \frac{1}{\rho e^{i\theta}} i\rho e^{i\theta}\, d\theta \right) = i a_{-1}(\theta_2 - \theta_1). \tag{24.63}$$

We note that result (24.60) is a special case of (24.63) in which θ_2 is equal to $\theta_1 + 2\pi$.

24.13 Definite integrals using contour integration

The remainder of this chapter is devoted to methods of applying contour integration and the residue theorem to various types of definite integral. However, three applications of contour integration, in which obtaining a value for the integral is not the prime purpose of the exercise, have been postponed until chapter 25. They are the location of the zeros of a complex polynomial, the evaluation of the sums of certain infinite series and the determination of inverse Laplace transforms.

For the integral evalations considered here, not much preamble is given since, for this material, the simplest explanation is felt to be via a series of worked examples that can be used as models.

24.13.1 Integrals of sinusoidal functions

Suppose that an integral of the form

$$\int_0^{2\pi} F(\cos\theta, \sin\theta)\, d\theta \tag{24.64}$$

is to be evaluated. It can be made into a contour integral around the unit circle C by writing $z = \exp i\theta$, and hence

$$\cos\theta = \tfrac{1}{2}(z + z^{-1}), \qquad \sin\theta = -\tfrac{1}{2}i(z - z^{-1}), \qquad d\theta = -iz^{-1}\, dz. \tag{24.65}$$

This contour integral can then be evaluated using the residue theorem, provided the transformed integrand has only a finite number of poles inside the unit circle and none on it.

►*Evaluate*

$$I = \int_0^{2\pi} \frac{\cos 2\theta}{a^2 + b^2 - 2ab\cos\theta}\, d\theta, \qquad b > a > 0. \tag{24.66}$$

By de Moivre's theorem (section 3.4),

$$\cos n\theta = \tfrac{1}{2}(z^n + z^{-n}). \tag{24.67}$$

Using $n = 2$ in (24.67) and straightforward substitution for the other functions of θ in (24.66) gives

$$I = \frac{i}{2ab} \oint_C \frac{z^4 + 1}{z^2(z - a/b)(z - b/a)}\, dz.$$

Thus there are two poles inside C, a double pole at $z = 0$ and a simple pole at $z = a/b$ (recall that $b > a$).

We could find the residue of the integrand at $z = 0$ by expanding the integrand as a Laurent series in z and identifying the coefficient of z^{-1}. Alternatively, we may use the

formula (24.56) with $m = 2$. Choosing the latter method and denoting the integrand by $f(z)$, we have

$$\frac{d}{dz}[z^2 f(z)] = \frac{d}{dz}\left[\frac{z^4+1}{(z-a/b)(z-b/a)}\right]$$
$$= \frac{(z-a/b)(z-b/a)4z^3 - (z^4+1)[(z-a/b)+(z-b/a)]}{(z-a/b)^2(z-b/a)^2}.$$

Now setting $z = 0$ and applying (24.56), we find

$$R(0) = \frac{a}{b} + \frac{b}{a}.$$

For the simple pole at $z = a/b$, equation (24.57) gives the residue as

$$R(a/b) = \lim_{z\to(a/b)}\left[(z-a/b)f(z)\right] = \frac{(a/b)^4+1}{(a/b)^2(a/b-b/a)}$$
$$= -\frac{a^4+b^4}{ab(b^2-a^2)}.$$

Therefore by the residue theorem

$$I = 2\pi i \times \frac{i}{2ab}\left[\frac{a^2+b^2}{ab} - \frac{a^4+b^4}{ab(b^2-a^2)}\right] = \frac{2\pi a^2}{b^2(b^2-a^2)}. \blacktriangleleft$$

24.13.2 Some infinite integrals

We next consider the evaluation of an integral of the form

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

where $f(z)$ has the following properties:

(i) $f(z)$ is analytic in the upper half-plane, $\operatorname{Im} z \geq 0$, except for a finite number of poles, none of which is on the real axis;
(ii) on a semicircle Γ of radius R (figure 24.14), R times the maximum of $|f|$ on Γ tends to zero as $R \to \infty$ (a sufficient condition is that $zf(z) \to 0$ as $|z| \to \infty$);
(iii) $\int_{-\infty}^{0} f(x)\,dx$ and $\int_{0}^{\infty} f(x)\,dx$ both exist.

Since

$$\left|\int_{\Gamma} f(z)\,dz\right| \leq 2\pi R \times (\text{maximum of } |f| \text{ on } \Gamma),$$

condition (ii) ensures that the integral along Γ tends to zero as $R \to \infty$, after which it is obvious from the residue theorem that the required integral is given by

$$\int_{-\infty}^{\infty} f(x)\,dx = 2\pi i \times (\text{sum of the residues at poles with } \operatorname{Im} z > 0). \tag{24.68}$$

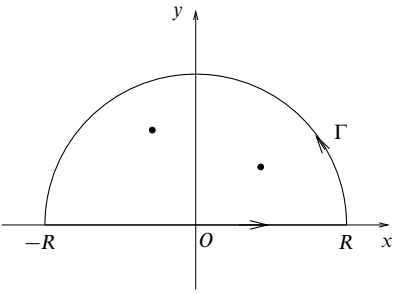


Figure 24.14 A semicircular contour in the upper half-plane.

►*Evaluate*

$$I = \int_0^\infty \frac{dx}{(x^2 + a^2)^4}, \qquad \textit{where } a \textit{ is real.}$$

The complex function $(z^2 + a^2)^{-4}$ has poles of order 4 at $z = \pm ai$, of which only $z = ai$ is in the upper half-plane. Conditions (ii) and (iii) are clearly satisfied. For higher-order poles, formula (24.56) for evaluating residues can be tiresome to apply. So, instead, we put $z = ai + \xi$ and expand for small ξ to obtain§

$$\frac{1}{(z^2 + a^2)^4} = \frac{1}{(2ai\xi + \xi^2)^4} = \frac{1}{(2ai\xi)^4}\left(1 - \frac{i\xi}{2a}\right)^{-4}.$$

The coefficient of ξ^{-1} is given by

$$\frac{1}{(2a)^4}\frac{(-4)(-5)(-6)}{3!}\left(\frac{-i}{2a}\right)^3 = \frac{-5i}{32a^7},$$

and hence by the residue theorem

$$\int_{-\infty}^{\infty} \frac{dx}{(x^2 + a^2)^4} = \frac{10\pi}{32a^7},$$

and so $I = 5\pi/(32a^7)$. ◄

Condition (i) of the previous method required there to be no poles of the integrand on the real axis, but in fact simple poles on the real axis can be accommodated by indenting the contour as shown in figure 24.15. The indentation at the pole $z = z_0$ is in the form of a semicircle γ of radius ρ in the upper half-plane, thus excluding the pole from the interior of the contour.

§ This illustrates another useful technique for determining residues.

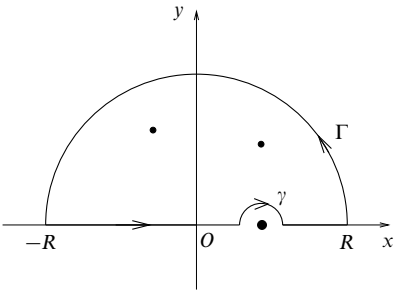


Figure 24.15 An indented contour used when the integrand has a simple pole on the real axis.

What is then obtained from a contour integration, apart from the contributions for Γ and γ, is called the *principal value of the integral,* defined as $\rho \to 0$ by

$$P\int_{-R}^{R} f(x)\,dx \equiv \int_{-R}^{z_0-\rho} f(x)\,dx + \int_{z_0+\rho}^{R} f(x)\,dx.$$

The remainder of the calculation goes through as before, but the contribution from the semicircle, γ, must be included. Result (24.63) of section 24.12 shows that since only a simple pole is involved its contribution is

$$-ia_{-1}\pi, \tag{24.69}$$

where a_{-1} is the residue at the pole and the minus sign arises because γ is traversed in the clockwise (negative) sense.

We defer giving an example of an indented contour until we have established *Jordan's lemma*; we will then work through an example illustrating both. Jordan's lemma enables infinite integrals involving sinusoidal functions to be evaluated.

For a function $f(z)$ of a complex variable z, if

(i) *$f(z)$ is analytic in the upper half-plane except for a finite number of poles in* $\operatorname{Im} z > 0$,
(ii) *the maximum of $|f(z)| \to 0$ as $|z| \to \infty$ in the upper half-plane,*
(iii) $m > 0$,

then

$$I_\Gamma = \int_\Gamma e^{imz} f(z)\,dz \to 0 \qquad \text{as } R \to \infty, \tag{24.70}$$

where Γ is the same semicircular contour as in figure 24.14.

Note that this condition (ii) is less stringent than the earlier condition (ii) (see the start of this section), since we now only require $M(R) \to 0$ and not $RM(R) \to 0$, where M is the maximum[§] of $|f(z)|$ on $|z| = R$.

[§] More strictly, the least upper bound.

The proof of the lemma is straightforward once it has been observed that, for $0 \le \theta \le \pi/2$,

$$1 \ge \frac{\sin\theta}{\theta} \ge \frac{2}{\pi}. \tag{24.71}$$

Then, since on Γ we have $|\exp(imz)| = |\exp(-mR\sin\theta)|$,

$$I_\Gamma \le \int_\Gamma |e^{imz} f(z)|\,|dz| \le MR\int_0^\pi e^{-mR\sin\theta}\,d\theta = 2MR\int_0^{\pi/2} e^{-mR\sin\theta}\,d\theta.$$

Thus, using (24.71),

$$I_\Gamma \le 2MR\int_0^{\pi/2} e^{-mR(2\theta/\pi)}\,d\theta = \frac{\pi M}{m}\left(1-e^{-mR}\right) < \frac{\pi M}{m};$$

hence, as $R\to\infty$, I_Γ tends to zero since M tends to zero.

►*Find the principal value of*

$$\int_{-\infty}^{\infty} \frac{\cos mx}{x-a}\,dx, \qquad \textit{for a real, } m>0.$$

Consider the function $(z-a)^{-1}\exp(imz)$; although it has no poles in the upper half-plane it does have a simple pole at $z=a$, and further $|(z-a)^{-1}|\to 0$ as $|z|\to\infty$. We will use a contour like that shown in figure 24.15 and apply the residue theorem. Symbolically,

$$\int_{-R}^{a-\rho} + \int_\gamma + \int_{a+\rho}^{R} + \int_\Gamma = 0. \tag{24.72}$$

Now as $R\to\infty$ and $\rho\to 0$ we have $\int_\Gamma \to 0$, by Jordan's lemma, and from (24.68) and (24.69) we obtain

$$P\int_{-\infty}^{\infty} \frac{e^{imx}}{x-a}\,dx - i\pi a_{-1} = 0, \tag{24.73}$$

where a_{-1} is the residue of $(z-a)^{-1}\exp(imz)$ at $z=a$, which is $\exp(ima)$. Then taking the real and imaginary parts of (24.73) gives

$$P\int_{-\infty}^{\infty} \frac{\cos mx}{x-a}\,dx = -\pi\sin ma, \qquad \text{as required,}$$

$$P\int_{-\infty}^{\infty} \frac{\sin mx}{x-a}\,dx = \pi\cos ma, \qquad \text{as a bonus.}\ ◄$$

24.13.3 Integrals of multivalued functions

We have discussed briefly some of the properties and difficulties associated with certain multivalued functions such as $z^{1/2}$ or $\mathrm{Ln}\,z$. It was mentioned that one method of managing such functions is by means of a 'cut plane'. A similar technique can be used with advantage to evaluate some kinds of infinite integral involving real functions for which the corresponding complex functions are multivalued. A typical contour employed for functions with a single branch point

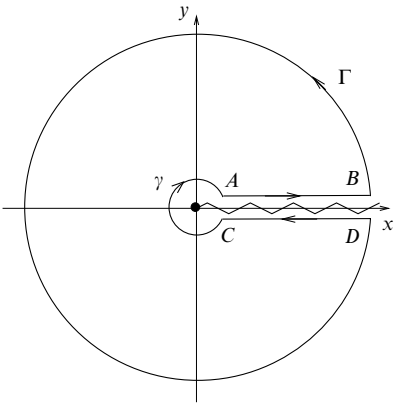


Figure 24.16 A typical cut-plane contour for use with multivalued functions that have a single branch point located at the origin.

located at the origin is shown in figure 24.16. Here Γ is a large circle of radius R and γ is a small one of radius ρ, both centred on the origin. Eventually we will let $R \to \infty$ and $\rho \to 0$.

The success of the method is due to the fact that because the integrand is multivalued, its values along the two lines AB and CD joining $z = \rho$ to $z = R$ are *not* equal and opposite although both are related to the corresponding real integral. Again an example provides the best explanation.

► *Evaluate*

$$I = \int_0^\infty \frac{dx}{(x+a)^3 x^{1/2}}, \qquad a > 0.$$

We consider the integrand $f(z) = (z+a)^{-3} z^{-1/2}$ and note that $|zf(z)| \to 0$ on the two circles as $\rho \to 0$ and $R \to \infty$. Thus the two circles make no contribution to the contour integral.

The only pole of the integrand inside the contour is at $z = -a$ (and is of order 3). To determine its residue we put $z = -a + \xi$ and expand (noting that $(-a)^{1/2}$ equals $a^{1/2}\exp(i\pi/2) = ia^{1/2}$):

$$\begin{aligned}\frac{1}{(z+a)^3 z^{1/2}} &= \frac{1}{\xi^3 i a^{1/2}(1-\xi/a)^{1/2}} \\ &= \frac{1}{i\xi^3 a^{1/2}}\left(1 + \frac{1}{2}\frac{\xi}{a} + \frac{3}{8}\frac{\xi^2}{a^2} + \cdots\right).\end{aligned}$$

The residue is thus $-3i/(8a^{5/2})$.

The residue theorem (24.61) now gives

$$\int_{AB} + \int_\Gamma + \int_{DC} + \int_\gamma = 2\pi i\left(\frac{-3i}{8a^{5/2}}\right).$$

We have seen that $\int_\Gamma$ and $\int_\gamma$ vanish, and if we denote z by x along the line AB then it has the value $z = x\exp 2\pi i$ along the line DC (note that $\exp 2\pi i$ must not be set equal to 1 until after the substitution for z has been made in $\int_{DC}$). Substituting these expressions,

$$\int_0^\infty \frac{dx}{(x+a)^3 x^{1/2}} + \int_\infty^0 \frac{dx}{[x\exp 2\pi i + a]^3 x^{1/2}\exp(\tfrac{1}{2}2\pi i)} = \frac{3\pi}{4a^{5/2}}.$$

Thus

$$\left(1 - \frac{1}{\exp \pi i}\right)\int_0^\infty \frac{dx}{(x+a)^3 x^{1/2}} = \frac{3\pi}{4a^{5/2}}$$

and

$$I = \frac{1}{2} \times \frac{3\pi}{4a^{5/2}}. \blacktriangleleft$$

Several other examples of integrals of multivalued functions around a variety of contours are included in the exercises that follow.

24.14 Exercises

24.1 Find an analytic function of $z = x + iy$ whose imaginary part is

$$(y\cos y + x\sin y)\exp x.$$

24.2 Find a function $f(z)$, analytic in a suitable part of the Argand diagram, for which

$$\text{Re } f = \frac{\sin 2x}{\cosh 2y - \cos 2x}.$$

Where are the singularities of $f(z)$?

24.3 Find the radii of convergence of the following Taylor series:

$$\text{(a)} \sum_{n=2}^{\infty} \frac{z^n}{\ln n}, \quad \text{(b)} \sum_{n=1}^{\infty} \frac{n!z^n}{n^n},$$
$$\text{(c)} \sum_{n=1}^{\infty} z^n n^{\ln n}, \quad \text{(d)} \sum_{n=1}^{\infty} \left(\frac{n+p}{n}\right)^{n^2} z^n, \text{ with } p \text{ real.}$$

24.4 Find the Taylor series expansion about the origin of the function $f(z)$ defined by

$$f(z) = \sum_{r=1}^{\infty} (-1)^{r+1} \sin\left(\frac{pz}{r}\right),$$

where p is a constant. Hence verify that $f(z)$ is a convergent series for all z.

24.5 Determine the types of singularities (if any) possessed by the following functions at $z = 0$ and $z = \infty$:

$$\text{(a) } (z-2)^{-1}, \quad \text{(b) } (1+z^3)/z^2, \quad \text{(c) } \sinh(1/z),$$
$$\text{(d) } e^z/z^3, \quad \text{(e) } z^{1/2}/(1+z^2)^{1/2}.$$

24.6 Identify the zeros, poles and essential singularities of the following functions:

$$\text{(a) } \tan z, \quad \text{(b) } [(z-2)/z^2]\sin[1/(1-z)], \quad \text{(c) } \exp(1/z),$$
$$\text{(d) } \tan(1/z), \quad \text{(e) } z^{2/3}.$$

24.7 Find the real and imaginary parts of the functions (i) z^2, (ii) e^z, and (iii) $\cosh \pi z$. By considering the values taken by these parts on the boundaries of the region $0 \leq x,\ y \leq 1$, determine the solution of Laplace's equation in that region that satisfies the boundary conditions

$$\phi(x,0) = 0, \qquad \phi(0,y) = 0,$$
$$\phi(x,1) = x, \qquad \phi(1,y) = y + \sin \pi y.$$

24.8 Show that the transformation

$$w = \int_0^z \frac{1}{(\zeta^3 - \zeta)^{1/2}}\, d\zeta$$

transforms the upper half-plane into the interior of a square that has one corner at the origin of the w-plane and sides of length L, where

$$L = \int_0^{\pi/2} \operatorname{cosec}^{1/2} \theta \; d\theta.$$

24.9 The *fundamental theorem of algebra* states that, for a complex polynomial $p_n(z)$ of degree n, the equation $p_n(z) = 0$ has precisely n complex roots. By applying Liouville's theorem (see the end of section 24.10) to $f(z) = 1/p_n(z)$, prove that $p_n(z) = 0$ has at least one complex root. Factor out that root to obtain $p_{n-1}(z)$ and, by repeating the process, prove the above theorem.

24.10 Show that, if a is a positive real constant, the function $\exp(iaz^2)$ is analytic and $\to 0$ as $|z| \to \infty$ for $0 < \arg z \leq \pi/4$. By applying Cauchy's theorem to a suitable contour prove that

$$\int_0^\infty \cos(ax^2)\, dx = \sqrt{\frac{\pi}{8a}}.$$

24.11 The function

$$f(z) = (1 - z^2)^{1/2}$$

of the complex variable z is defined to be real and positive on the real axis in the range $-1 < x < 1$. Using cuts running along the real axis for $1 < x < +\infty$ and $-\infty < x < -1$, show how $f(z)$ is made single-valued and evaluate it on the upper and lower sides of both cuts.

Use these results and a suitable contour in the complex z-plane to evaluate the integral

$$I = \int_1^\infty \frac{dx}{x(x^2 - 1)^{1/2}}.$$

Confirm your answer by making the substitution $x = \sec \theta$.

24.12 By considering the real part of

$$\int \frac{-iz^{n-1}\, dz}{1 - a(z + z^{-1}) + a^2},$$

where $z = \exp i\theta$ and n is a non-negative integer, evaluate

$$\int_0^\pi \frac{\cos n\theta}{1 - 2a\cos\theta + a^2}\, d\theta$$

for a real and > 1.

24.13 Prove that if $f(z)$ has a simple zero at z_0, then $1/f(z)$ has residue $1/f'(z_0)$ there. Hence evaluate

$$\int_{-\pi}^{\pi} \frac{\sin\theta}{a - \sin\theta}\, d\theta,$$

where a is real and > 1.

24.14 Prove that, for $\alpha > 0$, the integral

$$\int_0^\infty \frac{t \sin \alpha t}{1+t^2}\, dt$$

has the value $(\pi/2)\exp(-\alpha)$.

24.15 Prove that

$$\int_0^\infty \frac{\cos mx}{4x^4+5x^2+1}\, dx = \frac{\pi}{6}\left(4e^{-m/2} - e^{-m}\right) \qquad \text{for } m > 0.$$

24.16 Show that the principal value of the integral

$$\int_{-\infty}^\infty \frac{\cos(x/a)}{x^2-a^2}\, dx$$

is $-(\pi/a)\sin 1$.

24.17 The following is an alternative (and roundabout!) way of evaluating the Gaussian integral.

(a) Prove that the integral of $[\exp(i\pi z^2)]\operatorname{cosec} \pi z$ around the parallelogram with corners $\pm 1/2 \pm R\exp(i\pi/4)$ has the value $2i$.

(b) Show that the parts of the contour parallel to the real axis do not contribute when $R \to \infty$.

(c) Evaluate the integrals along the other two sides by putting $z' = r\exp(i\pi/4)$ and working in terms of $z' + \frac{1}{2}$ and $z' - \frac{1}{2}$. Hence, by letting $R \to \infty$ show that

$$\int_{-\infty}^\infty e^{-\pi r^2}\, dr = 1.$$

24.18 By applying the residue theorem around a wedge-shaped contour of angle $2\pi/n$, with one side along the real axis, prove that the integral

$$\int_0^\infty \frac{dx}{1+x^n},$$

where n is real and ≥ 2, has the value $(\pi/n)\operatorname{cosec}(\pi/n)$.

24.19 Using a suitable cut plane, prove that if α is real and $0 < \alpha < 1$ then

$$\int_0^\infty \frac{x^{-\alpha}}{1+x}\, dx$$

has the value $\pi \operatorname{cosec}\ \pi\alpha$.

24.20 Show that

$$\int_0^\infty \frac{\ln x}{x^{3/4}(1+x)}\, dx = -\sqrt{2}\pi^2.$$

24.21 By integrating a suitable function around a large semicircle in the upper half-plane and a small semicircle centred on the origin, determine the value of

$$I = \int_0^\infty \frac{(\ln x)^2}{1+x^2}\, dx$$

and deduce, as a by-product of your calculation, that

$$\int_0^\infty \frac{\ln x}{1+x^2}\, dx = 0.$$

24.22 The equation of an ellipse in plane polar coordinates r, θ, with one of its foci at the origin, is

$$\frac{l}{r} = 1 - \epsilon \cos\theta,$$

where l is a length (that of the latus rectum) and ϵ ($0 < \epsilon < 1$) is the eccentricity of the ellipse. Express the area of the ellipse as an integral around the unit circle in the complex plane, and show that the only singularity of the integrand inside the circle is a double pole at $z_0 = \epsilon^{-1} - (\epsilon^{-2} - 1)^{1/2}$.

By setting $z = z_0 + \xi$ and expanding the integrand in powers of ξ, find the residue at z_0 and hence show that the area is equal to $\pi l^2 (1 - \epsilon^2)^{-3/2}$.

[In terms of the semi-axes a and b of the ellipse, $l = b^2/a$ and $\epsilon^2 = (a^2 - b^2)/a^2$.]

24.15 Hints and answers

24.1 $\partial u/\partial y = -(\exp x)(y\cos y + x\sin y + \sin y)$; $z\exp z$.

24.3 (a) 1; (b) 1; (c) 1; (d) e^{-p}.

24.5 (a) Analytic, analytic; (b) double pole, single pole; (c) essential singularity, analytic; (d) triple pole, essential singularity; (e) branch point, branch point.

24.7 (i) $x^2 - y^2, 2xy$; (ii) $e^x \cos y, e^x \sin y$; (iii) $\cosh \pi x \cos \pi y, \sinh \pi x \sin \pi y$; $\phi(x, y) = xy + (\sinh \pi x \sin \pi y)/\sinh \pi$.

24.9 Assume that $p_r(x)$ ($r = n, n-1, \ldots, 1$) has no roots and then argue by the method of contradiction.

24.11 With $0 \le \theta_1 < 2\pi$ and $-\pi < \theta_2 \le \pi$, $f(z) = (r_1 r_2)^{1/2} \exp[\,i(\theta_1 + \theta_2 - \pi)\,]$. The four values are $\pm i(x^2 - 1)^{1/2}$, with the plus sign corresponding to points near the cut that lie in the second and fourth quadrants. $I = \pi/2$.

24.13 The only pole inside the unit circle is at $z = ia - i(a^2 - 1)^{1/2}$; the residue is given by $-(i/2)(a^2 - 1)^{-1/2}$; the integral has value $2\pi[a(a^2 - 1)^{-1/2} - 1]$.

24.15 Factorise the denominator, showing that the relevant simple poles are at $i/2$ and i.

24.17 (a) The only pole is at the origin with residue π^{-1};
(b) each is $\mathrm{O}[\exp(-\pi R^2 \mp \sqrt{2}\pi R)]$;
(c) the sum of the integrals is $2i \int_{-R}^{R} \exp(-\pi r^2)\, dr$.

24.19 Use a contour like that shown in figure 24.16.

24.21 Note that $\rho \ln^n \rho \to 0$ as $\rho \to 0$ for all n. When z is on the negative real axis, $(\ln z)^2$ contains three terms; one of the corresponding integrals is a standard form. The residue at $z = i$ is $i\pi^2/8$; $I = \pi^3/8$.

25

Applications of complex variables

In chapter 24, we developed the basic theory of the functions of a complex variable, $z = x + iy$, studied their analyticity (differentiability) properties and derived a number of results concerned with values of contour integrals in the complex plane. In this current chapter we will show how some of those results and properties can be exploited to tackle problems arising directly from physical situations or from apparently unrelated parts of mathematics.

In the former category will be the use of the differential properties of the real and imaginary parts of a function of a complex variable to solve problems involving Laplace's equation in two dimensions, whilst an example of the latter might be the summation of certain types of infinite series. Other applications, such as the Bromwich inversion formula for Laplace transforms, appear as mathematical problems that have their origins in physical applications; the Bromwich inversion enables us to extract the spatial or temporal response of a system to an initial input from the representation of that response in 'frequency space' – or, more correctly, imaginary frequency space.

Other topics that will be considered are the location of the (complex) zeros of a polynomial, the approximate evaluation of certain types of contour integrals using the methods of steepest descent and stationary phase, and the so-called 'phase-integral' solutions to some differential equations. For each of these a brief introduction is given at the start of the relevant section and to repeat them here would be pointless. We will therefore move on to our first topic of complex potentials.

25.1 Complex potentials

Towards the end of section 24.2 of the previous chapter it was shown that the real and the imaginary parts of an analytic function of z are separately solutions of Laplace's equation in two dimensions. Analytic functions thus offer a possible way

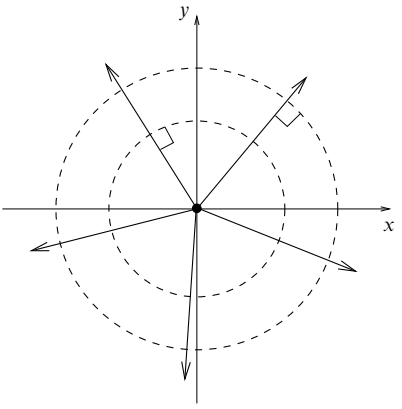


Figure 25.1 The equipotentials (dashed circles) and field lines (solid lines) for a line charge perpendicular to the z-plane.

of solving some two-dimensional physical problems describable by a potential satisfying $\nabla^2\phi = 0$. The general method is known as that of *complex potentials*.

We also found that if $f = u + iv$ is an analytic function of z then any curve $u =$ constant intersects any curve $v =$ constant at right angles. In the context of solutions of Laplace's equation, this result implies that the real and imaginary parts of $f(z)$ have an additional connection between them, for if the set of contours on which one of them is a constant represents the equipotentials of a system then the contours on which the other is constant, being orthogonal to each of the first set, must represent the *corresponding* field lines or stream lines, depending on the context. The analytic function f is the complex potential. It is conventional to use ϕ and ψ (rather than u and v) to denote the real and imaginary parts of a complex potential, so that $f = \phi + i\psi$.

As an example, consider the function

$$f(z) = \frac{-q}{2\pi\epsilon_0} \ln z \tag{25.1}$$

in connection with the physical situation of a line charge of strength q per unit length passing through the origin, perpendicular to the z-plane (figure 25.1). Its real and imaginary parts are

$$\phi = \frac{-q}{2\pi\epsilon_0} \ln |z|, \qquad \psi = \frac{-q}{2\pi\epsilon_0} \arg z. \tag{25.2}$$

The contours in the z-plane of $\phi =$ constant are concentric circles and those of $\psi =$ constant are radial lines. As expected these are orthogonal sets, but in addition they are, respectively, the equipotentials and electric field lines appropriate to

the field produced by the line charge. The minus sign is needed in (25.1) because the value of ϕ must decrease with increasing distance from the origin.

Suppose we make the choice that the real part ϕ of the analytic function f gives the conventional potential function; ψ could equally well be selected. Then we may consider how the direction and magnitude of the field are related to f.

►*Show that for any complex (electrostatic) potential $f(z)$ the strength of the electric field is given by $E = |f'(z)|$ and that its direction makes an angle of $\pi - \arg[f'(z)]$ with the x-axis.*

Because $\phi =$ constant is an equipotential, the field has components

$$E_x = -\frac{\partial \phi}{\partial x} \qquad \text{and} \qquad E_y = -\frac{\partial \phi}{\partial y}. \tag{25.3}$$

Since f is analytic, (i) we may use the Cauchy–Riemann relations (24.5) to change the second of these, obtaining

$$E_x = -\frac{\partial \phi}{\partial x} \qquad \text{and} \qquad E_y = \frac{\partial \psi}{\partial x}; \tag{25.4}$$

(ii) the direction of differentiation at a point is immaterial and so

$$\frac{df}{dz} = \frac{\partial f}{\partial x} = \frac{\partial \phi}{\partial x} + i\frac{\partial \psi}{\partial x} = -E_x + iE_y. \tag{25.5}$$

From these it can be seen that the field at a point is given in magnitude by $E = |f'(z)|$ and that it makes an angle with the x-axis given by $\pi - \arg[f'(z)]$. ◄

It will be apparent from the above that much of physical interest can be calculated by working directly in terms of f and z. In particular, the electric field vector $\mathbf{E}$ may be represented, using (25.5) above, by the quantity

$$\mathcal{E} = E_x + iE_y = -[f'(z)]^*.$$

Complex potentials can be used in two-dimensional fluid mechanics problems in a similar way. If the flow is stationary (i.e. the velocity of the fluid does not depend on time) and irrotational, and the fluid is both incompressible and non-viscous, then the velocity of the fluid can be described by $\mathbf{V} = \nabla\phi$, where ϕ is the velocity potential and satisfies $\nabla^2\phi = 0$. If, for a complex potential $f = \phi + i\psi$, the real part ϕ is taken to represent the velocity potential then the curves $\psi =$ constant will be the streamlines of the flow. In a direct parallel with the electric field, the velocity may be represented in terms of the complex potential by

$$\mathcal{V} = V_x + iV_y = [f'(z)]^*,$$

the difference of a minus sign reflecting the same difference between the definitions of $\mathbf{E}$ and $\mathbf{V}$. The speed of the flow is equal to $|f'(z)|$. Points where $f'(z) = 0$, and thus the velocity is zero, are called *stagnation points* of the flow.

Analogously to the electrostatic case, a line *source* of fluid at $z = z_0$, perpendicular to the z-plane (i.e. a point from which fluid is emerging at a constant rate),

is described by the complex potential

$$f(z) = k \ln(z - z_0),$$

where k is the strength of the source. A sink is similarly represented, but with k replaced by $-k$. Other simple examples are as follows.

(i) The flow of a fluid at a constant speed V_0 and at an angle α to the x-axis is described by $f(z) = V_0(\exp i\alpha)z$.

(ii) Vortex flow, in which fluid flows azimuthally in an anticlockwise direction around some point z_0, the speed of the flow being inversely proportional to the distance from z_0, is described by $f(z) = -ik \ln(z - z_0)$, where k is the strength of the vortex. For a clockwise vortex k is replaced by $-k$.

► *Verify that the complex potential*

$$f(z) = V_0 \left(z + \frac{a^2}{z} \right)$$

is appropriate to a circular cylinder of radius a placed so that it is perpendicular to a uniform fluid flow of speed V_0 parallel to the x-axis.

Firstly, since $f(z)$ is analytic except at $z = 0$, both its real and imaginary parts satisfy Laplace's equation in the region exterior to the cylinder. Also $f(z) \to V_0 z$ as $z \to \infty$, so that $\text{Re } f(z) \to V_0 x$, which is appropriate to a uniform flow of speed V_0 in the x-direction far from the cylinder.

Writing $z = r \exp i\theta$ and using de Moivre's theorem we have

$$\begin{aligned} f(z) &= V_0 \left[r \exp i\theta + \frac{a^2}{r} \exp(-i\theta) \right] \\ &= V_0 \left(r + \frac{a^2}{r} \right) \cos\theta + iV_0 \left(r - \frac{a^2}{r} \right) \sin\theta. \end{aligned}$$

Thus we see that the streamlines of the flow described by $f(z)$ are given by

$$\psi = V_0 \left(r - \frac{a^2}{r} \right) \sin\theta = \text{constant}.$$

In particular, $\psi = 0$ on $r = a$, independently of the value of θ, and so $r = a$ must be a streamline. Since there can be no flow of fluid across streamlines, $r = a$ must correspond to a boundary along which the fluid flows tangentially. Thus $f(z)$ is a solution of Laplace's equation that satisfies all the physical boundary conditions of the problem, and so, by the uniqueness theorem, it is the appropriate complex potential. ◄

By a similar argument, the complex potential $f(z) = -E(z - a^2/z)$ (note the minus signs) is appropriate to a conducting circular cylinder of radius a placed perpendicular to a uniform electric field $\mathbf{E}$ in the x-direction.

The real and imaginary parts of a complex potential $f = \phi + i\psi$ have another interesting relationship in the context of Laplace's equation in electrostatics or fluid mechanics. Let us choose ϕ as the conventional potential, so that ψ represents the stream function (or electric field, depending on the application), and consider

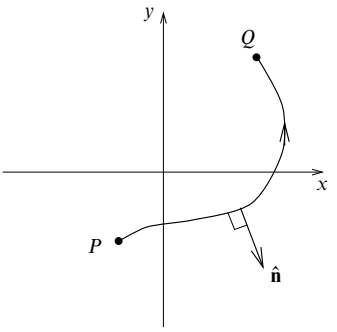


Figure 25.2 A curve joining the points P and Q. Also shown is $\hat{\mathbf{n}}$, the unit vector normal to the curve.

the difference in the values of ψ at any two points P and Q connected by some path C, as shown in figure 25.2. This difference is given by

$$\psi(Q) - \psi(P) = \int_P^Q d\psi = \int_P^Q \left(\frac{\partial \psi}{\partial x}\, dx + \frac{\partial \psi}{\partial y}\, dy \right),$$

which, on using the Cauchy–Riemann relations, becomes

$$\begin{aligned} \psi(Q) - \psi(P) &= \int_P^Q \left(-\frac{\partial \phi}{\partial y}\, dx + \frac{\partial \phi}{\partial x}\, dy \right) \\ &= \int_P^Q \nabla\phi \cdot \hat{\mathbf{n}}\, ds \;=\; \int_P^Q \frac{\partial \phi}{\partial n}\, ds, \end{aligned}$$

where $\hat{\mathbf{n}}$ is the vector unit normal to the path C and s is the arc length along the path; the last equality is written in terms of the normal derivative $\partial\phi/\partial n \equiv \nabla\phi \cdot \hat{\mathbf{n}}$.

Now suppose that in an electrostatics application, the path C is the surface of a conductor; then

$$\frac{\partial \phi}{\partial n} = -\frac{\sigma}{\epsilon_0},$$

where σ is the surface charge density per unit length normal to the xy-plane. Therefore $-\epsilon_0[\psi(Q) - \psi(P)]$ is equal to the charge per unit length normal to the xy-plane on the surface of the conductor between the points P and Q. Similarly, in fluid mechanics applications, if the density of the fluid is ρ and its velocity is $\mathbf{V}$ then

$$\rho[\psi(Q) - \psi(P)] = \rho \int_P^Q \nabla\phi \cdot \hat{\mathbf{n}}\, ds = \rho \int_P^Q \mathbf{V} \cdot \hat{\mathbf{n}}\, ds$$

is equal to the mass flux between P and Q per unit length perpendicular to the xy-plane.

► *A conducting circular cylinder of radius a is placed with its centre line passing through the origin and perpendicular to a uniform electric field* **E** *in the x-direction. Find the charge per unit length induced on the half of the cylinder that lies in the region* $x < 0$.

As mentioned immediately following the previous example, the appropriate complex potential for this problem is $f(z) = -E(z - a^2/z)$. Writing $z = r\exp i\theta$ this becomes

$$\begin{aligned} f(z) &= -E\left[r\exp i\theta - \frac{a^2}{r}\exp(-i\theta)\right] \\ &= -E\left(r - \frac{a^2}{r}\right)\cos\theta - iE\left(r + \frac{a^2}{r}\right)\sin\theta, \end{aligned}$$

so that on $r = a$ the imaginary part of f is given by

$$\psi = -2Ea\sin\theta.$$

Therefore the induced charge q per unit length on the left half of the cylinder, between $\theta = \pi/2$ and $\theta = 3\pi/2$, is given by

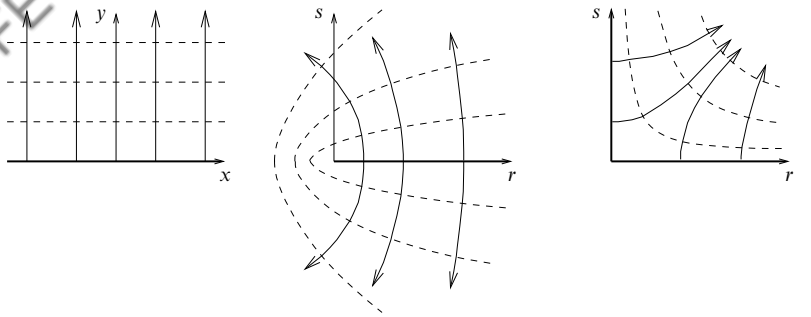
$$q = 2\epsilon_0 Ea[\sin(3\pi/2) - \sin(\pi/2)] = -4\epsilon_0 Ea. \text{ ◄}$$

25.2 Applications of conformal transformations

In section 24.7 of the previous chapter it was shown that, under a conformal transformation $w = g(z)$ from $z = x+iy$ to a new variable $w = r+is$, if a solution of Laplace's equation in some region R of the xy-plane can be found as the real or imaginary part of an analytic function[§] of z, then the same expression put in terms of r and s will be a solution of Laplace's equation in the corresponding region R' of the w-plane, and vice versa. In addition, if the solution is constant over the boundary C of the region R in the xy-plane, then the solution in the w-plane will take the same constant value over the corresponding curve C' that bounds R'.

Thus, from any two-dimensional solution of Laplace's equation for a particular geometry, typified by those discussed in the previous section, further solutions for other geometries can be obtained by making conformal transformations. From the physical point of view the given geometry is usually complicated, and so the solution is sought by transforming to a simpler one. However, working from simpler to more complicated situations can provide useful experience and make it more likely that the reverse procedure can be tackled successfully.

[§] In fact, the original solution in the xy-plane need not be given explicitly as the real or imaginary part of an analytic function. Any solution of $\nabla^2\phi = 0$ in the xy-plane is carried over into another solution of $\nabla^2\phi = 0$ in the new variables by a conformal transformation, and vice versa.



(a) z-plane (b) w-plane (c) w-plane

Figure 25.3 The equipotential lines (broken) and field lines (solid) (a) for an infinite charged conducting plane at $y = 0$, where $z = x + iy$, and after the transformations (b) $w = z^2$ and (c) $w = z^{1/2}$ of the situation shown in (a).

► *Find the complex electrostatic potential associated with an infinite charged conducting plate $y = 0$, and thus obtain those associated with*
(i) *a semi-infinite charged conducting plate ($r > 0$, $s = 0$);*
(ii) *the inside of a right-angled charged conducting wedge ($r > 0$, $s = 0$ and $r = 0$, $s > 0$).*

Figure 25.3(a) shows the equipotentials (broken lines) and field lines (solid lines) for the infinite charged conducting plane $y = 0$. Suppose that we elect to make the real part of the complex potential coincide with the conventional electrostatic potential. If the plate is charged to a potential V then clearly

$$\phi(x, y) = V - ky, \tag{25.6}$$

where k is related to the charge density σ by $k = \sigma/\epsilon_0$, since physically the electric field $\mathbf{E}$ has components $(0, \sigma/\epsilon_0)$ and $\mathbf{E} = -\nabla\phi$.

Thus what is needed is an analytic function of z, of which the real part is $V - ky$. This can be obtained by inspection, but we may proceed formally and use the Cauchy–Riemann relations to obtain the imaginary part $\psi(x, y)$ as follows:

$$\frac{\partial\psi}{\partial y} = \frac{\partial\phi}{\partial x} = 0 \qquad \text{and} \qquad \frac{\partial\psi}{\partial x} = -\frac{\partial\phi}{\partial y} = k.$$

Hence $\psi = kx + c$ and, absorbing c into V, the required complex potential is

$$f(z) = V - ky + ikx = V + ikz. \tag{25.7}$$

(i) Now consider the transformation

$$w = g(z) = z^2. \tag{25.8}$$

This satisfies the criteria for a conformal mapping (except at $z = 0$) and carries the upper half of the z-plane into the entire w-plane; the equipotential plane $y = 0$ goes into the half-plane $r > 0$, $s = 0$.

By the general results proved, $f(z)$, when expressed in terms of r and s, will give a complex potential whose real part will be constant on the half-plane in question; we

deduce that

$$F(w) = f(z) = V + ikz = V + ikw^{1/2} \tag{25.9}$$

is the required potential. Expressed in terms of r, s and $\rho = (r^2 + s^2)^{1/2}$, $w^{1/2}$ is given by

$$w^{1/2} = \rho^{1/2}\left[\left(\frac{\rho + r}{2\rho}\right)^{1/2} + i\left(\frac{\rho - r}{2\rho}\right)^{1/2}\right], \tag{25.10}$$

and, in particular, the electrostatic potential is given by

$$\Phi(r, s) = \operatorname{Re} F(w) = V - \frac{k}{\sqrt{2}}\left[(r^2 + s^2)^{1/2} - r\right]^{1/2}. \tag{25.11}$$

The corresponding equipotentials and field lines are shown in figure 25.3(b). Using results (25.3)–(25.5), the magnitude of the electric field is

$$|\mathbf{E}| = |F'(w)| = |\tfrac{1}{2}ikw^{-1/2}| = \tfrac{1}{2}k(r^2 + s^2)^{-1/4}.$$

(ii) A transformation 'converse' to that used in (i),

$$w = g(z) = z^{1/2},$$

has the effect of mapping the upper half of the z-plane into the first quadrant of the w-plane and the conducting plane $y = 0$ into the wedge $r > 0$, $s = 0$ and $r = 0$, $s > 0$.

The complex potential now becomes

$$\begin{aligned} F(w) &= V + ikw^2 \\ &= V + ik[(r^2 - s^2) + 2irs], \end{aligned} \tag{25.12}$$

showing that the electrostatic potential is $V - 2krs$ and that the electric field has components

$$\mathbf{E} = (2ks, 2kr). \tag{25.13}$$

Figure 25.3(c) indicates the approximate equipotentials and field lines. (Note that, in both transformations, $g'(z)$ is either 0 or ∞ at the origin, and so neither transformation is conformal there. Consequently there is no violation of result (ii), given at the start of section 24.7, concerning the angles between intersecting lines.) ◄

The *method of images*, discussed in section 21.5, can be used in conjunction with conformal transformations to solve some problems involving Laplace's equation in two dimensions.

►*A wedge of angle π/α with its vertex at $z = 0$ is formed by two semi-infinite conducting plates, as shown in figure 25.4*(a). *A line charge of strength q per unit length is positioned at $z = z_0$, perpendicular to the z-plane. By considering the transformation $w = z^\alpha$, find the complex electrostatic potential for this situation.*

Let us consider the action of the transformation $w = z^\alpha$ on the lines defining the positions of the conducting plates. The plate that lies along the positive x-axis is mapped onto the positive r-axis in the w-plane, whereas the plate that lies along the direction $\exp(i\pi/\alpha)$ is mapped into the negative r-axis, as shown in figure 25.4(b). Similarly the line charge at z_0 is mapped onto the point $w_0 = z_0^\alpha$.

From figure 25.4(b), we see that in the w-plane the problem can be solved by introducing a second line charge of opposite sign at the point w_0^*, so that the potential $\Phi = 0$ along the r-axis. The complex potential for such an arrangement is simply

$$F(w) = -\frac{q}{2\pi\epsilon_0}\ln(w - w_0) + \frac{q}{2\pi\epsilon_0}\ln(w - w_0^*).$$

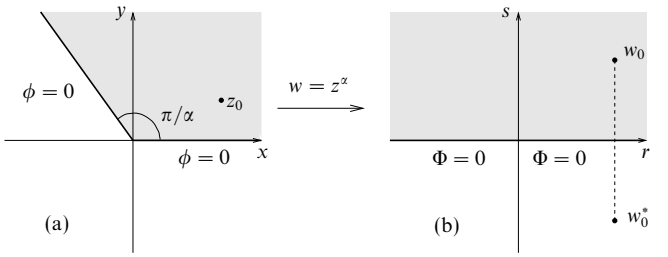


Figure 25.4 (a) An infinite conducting wedge with interior angle π/α and a line charge at $z = z_0$; (b) after the transformation $w = z^\alpha$, with an additional image charge placed at $w = w_0^*$.

Substituting $w = z^\alpha$ into the above shows that the required complex potential in the original z-plane is

$$f(z) = \frac{q}{2\pi\epsilon_0} \ln\left(\frac{z^\alpha - z_0^{*\alpha}}{z^\alpha - z_0^\alpha}\right). \blacktriangleleft$$

It should be noted that the appearance of a complex conjugate in the final expression is not in conflict with the general requirement that the complex potential be analytic. It is z^* that must not appear; here, $z_0^{*\alpha}$ is no more than a parameter of the problem.

25.3 Location of zeros

The residue theorem, relating the value of a closed contour integral to the sum of the residues at the poles enclosed by the contour, was discussed in the previous chapter. One important practical use of an extension to the theorem is that of locating the zeros of functions of a complex variable. The location of such zeros has a particular application in electrical network and general oscillation theory, since the complex zeros of certain functions (usually polynomials) give the system parameters (usually frequencies) at which system instabilities occur. As the basis of a method for locating these zeros we next prove three important theorems.

(i) If $f(z)$ has poles as its only singularities inside a closed contour C and is not zero at any point on C then

$$\oint_C \frac{f'(z)}{f(z)}\, dz = 2\pi i \sum_j (N_j - P_j). \tag{25.14}$$

Here N_j is the order of the jth zero of $f(z)$ enclosed by C. Similarly P_j is the order of the jth pole of $f(z)$ inside C.

To prove this we note that, at each position z_j, $f(z)$ can be written as

$$f(z) = (z - z_j)^{m_j} \phi(z), \tag{25.15}$$

where $\phi(z)$ is analytic and non-zero at $z = z_j$ and m_j is positive for a zero and negative for a pole. Then the integrand $f'(z)/f(z)$ takes the form

$$\frac{f'(z)}{f(z)} = \frac{m_j}{z - z_j} + \frac{\phi'(z)}{\phi(z)}. \tag{25.16}$$

Since $\phi(z_j) \neq 0$, the second term on the RHS is analytic; thus the integrand has a simple pole at $z = z_j$, with residue m_j. For zeros $m_j = N_j$ and for poles $m_j = -P_j$, and thus (25.14) follows from the residue theorem.

(ii) If $f(z)$ is analytic inside C and not zero at any point on it then

$$2\pi \sum_j N_j = \Delta_C[\arg f(z)], \tag{25.17}$$

where $\Delta_C[x]$ denotes the variation in x around the contour C.

Since f is analytic, there are no P_j; further, since

$$\frac{f'(z)}{f(z)} = \frac{d}{dz}[\operatorname{Ln} f(z)], \tag{25.18}$$

equation (25.14) can be written

$$2\pi i \sum N_j = \oint_C \frac{f'(z)}{f(z)}\, dz = \Delta_C[\operatorname{Ln} f(z)]. \tag{25.19}$$

However,

$$\Delta_C[\operatorname{Ln} f(z)] = \Delta_C[\ln |f(z)|] + i\Delta_C[\arg f(z)], \tag{25.20}$$

and, since C is a closed contour, $\ln |f(z)|$ must return to its original value; so the real term on the RHS is zero. Comparison of (25.19) and (25.20) then establishes (25.17), which is known as the *principle of the argument*.

(iii) If $f(z)$ and $g(z)$ are analytic within and on a closed contour C and $|g(z)| < |f(z)|$ on C then $f(z)$ and $f(z) + g(z)$ have the same number of zeros inside C; this is *Rouché's theorem.*

With the conditions given, neither $f(z)$ nor $f(z) + g(z)$ can have a zero on C. So, applying theorem (ii) with an obvious notation,

$$\begin{aligned} 2\pi \textstyle\sum_j N_j(f+g) &= \Delta_C[\arg(f+g)] \\ &= \Delta_C[\arg f] + \Delta_C[\arg(1 + g/f)] \\ &= 2\pi \textstyle\sum_k N_k(f) + \Delta_C[\arg(1 + g/f)]. \end{aligned} \tag{25.21}$$

Further, since $|g| < |f|$ on C, $1 + g/f$ always lies *within* a unit circle centred on $z = 1$; thus its argument *always* lies in the range $-\pi/2 < \arg(1 + g/f) < \pi/2$ and cannot change by any multiple of 2π. It must therefore return to its original value when z returns to its starting point having traversed C. Hence the second term on the RHS of (25.21) is zero and the theorem is established.

The importance of Rouché's theorem is that for some functions, in particular

polynomials, only the behaviour of a single term in the function need be considered if the contour is chosen appropriately. For example, for a polynomial, $f(z)+g(z)=\sum_0^N b_i z^i$, only the properties of its largest power, taken as $f(z)$, need be investigated if a circular contour is chosen with radius R sufficiently large that, on the contour, the magnitude of the largest power term, $|b_N R^N|$, is greater than the sum of the magnitudes of all other terms. It is obvious that $f(z)=b_N z^N$ has N zeros inside $|z|=R$ (all at the origin); consequently, $f+g$ also has N zeros inside the same circle.

The corresponding situation, in which only the properties of the polynomial's smallest power, again taken as $f(z)$, need be investigated is a circular contour with a radius R chosen sufficiently *small* that, on the contour, the magnitude of the smallest power term (usually the constant term in a polynomial) is greater than the sum of the magnitudes of all other terms. Then, a similar argument to that given above shows that, since $f(z)=b_0$ has no zeros inside $|z|=R$, neither does $f+g$.

A weak form of the *maximum-modulus theorem* may also be deduced. This states that if $f(z)$ is analytic within and on a simple closed contour C then $|f(z)|$ attains its maximum value on the boundary of C. The proof is as follows.

Let $|f(z)|\leq M$ on C with equality at at least one point of C. Now suppose that there is a point $z=a$ inside C such that $|f(a)|>M$. Then the function $h(z)\equiv f(a)$ is such that $|h(z)|>|-f(z)|$ on C, and thus, by Rouché's theorem, $h(z)$ and $h(z)-f(z)$ have the same number of zeros inside C. But $h(z)$ $(\equiv f(a))$ has no zeros inside C, and, again by Rouché's theorem, this would imply that $f(a)-f(z)$ has no zeros in C. However, $f(a)-f(z)$ clearly has a zero at $z=a$, and so we have a contradiction; the assumption of the existence of a point $z=a$ inside C such that $|f(a)|>M$ must be invalid. This establishes the theorem.

The stronger form of the maximum-modulus theorem, which we do not prove, states, in addition, that the maximum value of $f(z)$ is not attained at any interior point except for the case where $f(z)$ is a constant.

► *Show that the four zeros of $h(z)=z^4+z+1$ occur one in each quadrant of the Argand diagram and that all four lie between the circles $|z|=2/3$ and $|z|=3/2$.*

Putting $z=x$ and $z=iy$ shows that no zeros occur on the real or imaginary axes. They must therefore occur in conjugate pairs, as can be shown by taking the complex conjugate of $h(z)=0$.

Now take C as the contour $OXYO$ shown in figure 25.5 and consider the changes $\Delta[\arg h]$ in the argument of $h(z)$ as z traverses C.

(i) OX: $\arg h$ is everywhere zero, since h is real, and thus $\Delta_{OX}[\arg h]=0$.
(ii) XY: $z=R\exp i\theta$ and so $\arg h$ changes by an amount

$$\begin{aligned}\Delta_{XY}[\arg h] &= \Delta_{XY}[\arg z^4]+\Delta_{XY}[\arg(1+z^{-3}+z^{-4})]\\ &= \Delta_{XY}[\arg R^4 e^{4i\theta}]+\Delta_{XY}\left\{\arg[1+\mathrm{O}(R^{-3})]\right\}\\ &= 2\pi+\mathrm{O}(R^{-3}).\end{aligned}\tag{25.22}$$

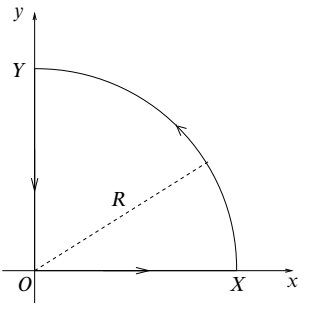


Figure 25.5 A contour for locating the zeros of a polynomial that occur in the first quadrant of the Argand diagram.

(iii) YO: $z = iy$ and so $\arg h = \tan^{-1} y/(y^4 + 1)$, which starts at $O(R^{-3})$ and finishes at 0 as y goes from large R to 0. It never reaches $\pi/2$ because $y^4 + 1 = 0$ has no real positive root. Thus $\Delta_{YO}[\arg h] = 0$.

Hence for the complete contour $\Delta_C[\arg h] = 0 + 2\pi + 0 + O(R^{-3})$, and, if R is allowed to tend to infinity, we deduce from (25.17) that $h(z)$ has one zero in the first quadrant. Furthermore, since the roots occur in conjugate pairs, a second root must lie in the fourth quadrant, and the other pair must lie in the second and third quadrants.

To show that the zeros lie within the given annulus in the z-plane we apply Rouché's theorem, as follows.

(i) With C as $|z| = 3/2$, $f = z^4$, $g = z + 1$. Now $|f| = 81/16$ on C and $|g| \leq 1 + |z| < 5/2 < 81/16$. Thus, since $z^4 = 0$ has four roots inside $|z| = 3/2$, so also does $z^4 + z + 1 = 0$.

(ii) With C as $|z| = 2/3$, $f = 1$, $g = z^4 + z$. Now $f = 1$ on C and $|g| \leq |z^4| + |z| = 16/81 + 2/3 = 70/81 < 1$. Thus, since $f = 0$ has no roots inside $|z| = 2/3$, neither does $1 + z + z^4 = 0$.

Hence the four zeros of $h(z) = z^4 + z + 1$ occur one in each quadrant and all lie between the circles $|z| = 2/3$ and $|z| = 3/2$. ◄

A further technique useful for locating the zeros of functions is explained in exercise 25.8.

25.4 Summation of series

We now turn to an application of contour integration which at first sight might seem to lie in an unrelated area of mathematics, namely the summation of infinite series. Sometimes a real infinite series with index n, say, can be summed with the help of a suitable complex function that has poles on the real axis at the various positions $z = n$ with the corresponding residues at those poles equal to the values of the terms of the series. A worked example provides the best explanation of how the technique is applied; other examples will be found in the exercises.

►*By considering*

$$\oint_C \frac{\pi \cot \pi z}{(a+z)^2}\, dz,$$

where a is not an integer and C is a circle of large radius, evaluate

$$\sum_{n=-\infty}^{\infty} \frac{1}{(a+n)^2}.$$

The integrand has (i) simple poles at $z =$ integer n, for $-\infty < n < \infty$, due to the factor $\cot \pi z$ and (ii) a double pole at $z = -a$.

(i) To find the residue of $\cot \pi z$, put $z = n + \xi$ for small ξ:

$$\cot \pi z = \frac{\cos(n\pi + \xi\pi)}{\sin(n\pi + \xi\pi)} \approx \frac{\cos n\pi}{(\cos n\pi)\xi\pi} = \frac{1}{\xi\pi}.$$

The residue of the integrand at $z = n$ is thus $\pi(a+n)^{-2}\pi^{-1}$.

(ii) Putting $z = -a + \xi$ for small ξ and determining the coefficient of ξ^{-1} gives[§]

$$\begin{aligned}\frac{\pi \cot \pi z}{(a+z)^2} &= \frac{\pi}{\xi^2} \cot(-a\pi + \xi\pi) \\ &= \frac{\pi}{\xi^2} \left\{ \cot(-a\pi) + \xi \left[\frac{d}{dz}(\cot \pi z) \right]_{z=-a} + \cdots \right\},\end{aligned}$$

so that the residue at the double pole $z = -a$ is given by

$$\pi[-\pi \operatorname{cosec}^2 \pi z]_{z=-a} = -\pi^2 \operatorname{cosec}^2 \pi a.$$

Collecting together these results to express the residue theorem gives

$$I = \oint_C \frac{\pi \cot \pi z}{(a+z)^2}\, dz = 2\pi i \left[\sum_{n=-N}^{N} \frac{1}{(a+n)^2} - \pi^2 \operatorname{cosec}^2 \pi a \right], \tag{25.23}$$

where N equals the integer part of R. But as the radius R of C tends to ∞, $\cot \pi z \to \mp i$ (depending on whether Im z is greater or less than zero, respectively). Thus

$$I < k \int \frac{dz}{(a+z)^2},$$

which tends to 0 as $R \to \infty$. Thus $I \to 0$ as R (and hence N) $\to \infty$, and (25.23) establishes the result

$$\sum_{n=-\infty}^{\infty} \frac{1}{(a+n)^2} = \frac{\pi^2}{\sin^2 \pi a}. \blacktriangleleft$$

Series with alternating signs in the terms, i.e. $(-1)^n$, can also be attempted in this way but using $\operatorname{cosec} \pi z$ rather than $\cot \pi z$, since the former has residue $(-1)^n \pi^{-1}$ at $z = n$ (see exercise 25.11).

[§] This again illustrates one of the techniques for determining residues.

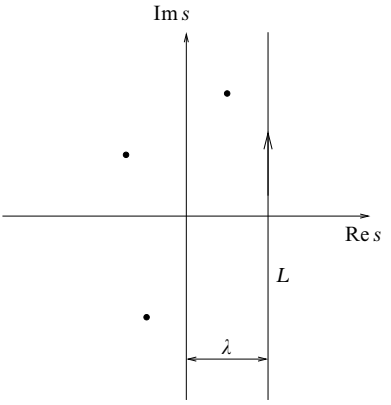


Figure 25.6 The integration path of the inverse Laplace transform is along the infinite line L. The quantity λ must be positive and large enough for all poles of the integrand to lie to the left of L.

25.5 Inverse Laplace transform

As a further example of the use of contour integration we now discuss a method whereby the process of Laplace transformation, discussed in chapter 13, can be inverted.

It will be recalled that the Laplace transform $\bar{f}(s)$ of a function $f(x)$, $x \geq 0$, is given by

$$\bar{f}(s) = \int_0^\infty e^{-sx} f(x)\, dx, \qquad \text{Re } s > s_0. \tag{25.24}$$

In chapter 13, functions $f(x)$ were deduced from the transforms by means of a prepared dictionary. However, an explicit formula for an unknown inverse may be written in the form of an integral. It is known as the *Bromwich integral* and is given by

$$f(x) = \frac{1}{2\pi i} \int_{\lambda - i\infty}^{\lambda + i\infty} e^{sx} \bar{f}(s)\, ds, \qquad \lambda > 0, \tag{25.25}$$

where s is treated as a complex variable and the integration is along the line L indicated in figure 25.6. The position of the line is dictated by the requirements that λ is positive and that all singularities of $\bar{f}(s)$ lie to the left of the line.

That (25.25) really is the unique inverse of (25.24) is difficult to show for general functions and transforms, but the following verification should at least make it

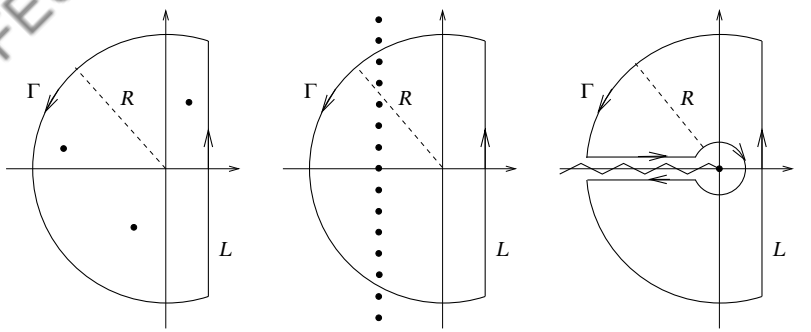


Figure 25.7 Some contour completions for the integration path L of the inverse Laplace transform. For details of when each is appropriate see the main text.

plausible:

$$\begin{aligned} f(x) &= \frac{1}{2\pi i}\int_{\lambda-i\infty}^{\lambda+i\infty} ds\, e^{sx}\int_0^\infty e^{-su}f(u)\,du, \qquad \mathrm{Re}(s)>0,\ \text{i.e. } \lambda>0,\\ &= \frac{1}{2\pi i}\int_0^\infty du\, f(u)\int_{\lambda-i\infty}^{\lambda+i\infty} e^{s(x-u)}\,ds\\ &= \frac{1}{2\pi i}\int_0^\infty du\, f(u)\int_{-\infty}^{\infty} e^{\lambda(x-u)}e^{ip(x-u)}i\,dp, \qquad \text{putting } s=\lambda+ip,\\ &= \frac{1}{2\pi}\int_0^\infty f(u)e^{\lambda(x-u)}2\pi\delta(x-u)\,du\\ &= \begin{cases} f(x) & x\geq 0,\\ 0 & x<0. \end{cases} \end{aligned} \tag{25.26}$$

Our main purpose here is to demonstrate the use of contour integration. To employ it in the evaluation of the line integral (25.25), the path L must be made part of a closed contour in such a way that the contribution from the completion either vanishes or is simply calculable.

A typical completion is shown in figure 25.7(a) and would be appropriate if $\bar{f}(s)$ had a finite number of poles. For more complicated cases, in which $\bar{f}(s)$ has an infinite sequence of poles but all to the left of L as in figure 25.7(b), a sequence of circular-arc completions that pass between the poles must be used and $f(x)$ is obtained as a series. If $\bar{f}(s)$ is a multivalued function then a cut plane is needed and a contour such as that shown in figure 25.7(c) might be appropriate.

We consider here only the simple case in which the contour in figure 25.7(a) is used; we refer the reader to the exercises at the end of the chapter for others.

Ideally, we would like the contribution to the integral from the circular arc Γ to tend to zero as its radius $R \to \infty$. Using a modified version of Jordan's lemma, it may be shown that this is indeed the case if there exist constants $M > 0$ and $\alpha > 0$ such that on Γ

$$|\bar{f}(s)| \leq \frac{M}{R^{\alpha}}.$$

Moreover, this condition always holds when $\bar{f}(s)$ has the form

$$\bar{f}(s) = \frac{P(s)}{Q(s)},$$

where $P(s)$ and $Q(s)$ are polynomials and the degree of $Q(s)$ is greater than that of $P(s)$.

When the contribution from the part-circle Γ tends to zero as $R \to \infty$, we have from the residue theorem that the inverse Laplace transform (25.25) is given simply by

$$f(t) = \sum \left(\text{residues of } \bar{f}(s)e^{sx} \text{ at all poles}\right). \tag{25.27}$$

►*Find the function $f(x)$ whose Laplace transform is*

$$\bar{f}(s) = \frac{s}{s^2 - k^2},$$

where k is a constant.

It is clear that $\bar{f}(s)$ is of the form required for the integral over the circular arc Γ to tend to zero as $R \to \infty$, and so we may use the result (25.27) directly. Now

$$\bar{f}(s)e^{sx} = \frac{se^{sx}}{(s-k)(s+k)},$$

and thus has simple poles at $s = k$ and $s = -k$. Using (24.57) the residues at each pole can be easily calculated as

$$R(k) = \frac{ke^{kx}}{2k} \qquad \text{and} \qquad R(-k) = \frac{ke^{-kx}}{2k}.$$

Thus the inverse Laplace transform is given by

$$f(x) = \tfrac{1}{2}\left(e^{kx} + e^{-kx}\right) = \cosh kx.$$

This result may be checked by computing the forward transform of $\cosh kx$. ◄

Sometimes a little more care is required when deciding in which half-plane to close the contour C.

►*Find the function $f(x)$ whose Laplace transform is*

$$\bar{f}(s) = \frac{1}{s}(e^{-as} - e^{-bs}),$$

where a and b are fixed and positive, with $b > a$.

From (25.25) we have the integral

$$f(x) = \frac{1}{2\pi i}\int_{\lambda - i\infty}^{\lambda + i\infty} \frac{e^{(x-a)s} - e^{(x-b)s}}{s}\, ds. \tag{25.28}$$

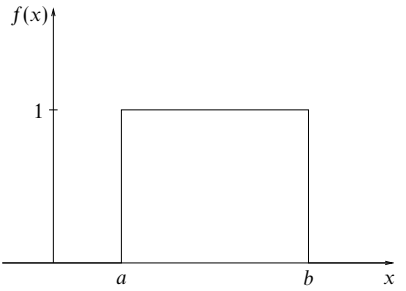


Figure 25.8 The result of the Laplace inversion of $\bar{f}(s) = s^{-1}(e^{-as} - e^{-bs})$ with $b > a$.

Now, despite appearances to the contrary, the integrand has no poles, as may be confirmed by expanding the exponentials as Taylor series about $s = 0$. Depending on the value of x, several cases arise.

(i) For $x < a$ both exponentials in the integrand will tend to zero as Re $s \to \infty$. Thus we may close L with a circular arc Γ in the *right* half-plane (λ can be as small as desired), and we observe that $s \times$ integrand tends to zero everywhere on Γ as $R \to \infty$. With no poles enclosed and no contribution from Γ, the integral along L must also be zero. Thus

$$f(x) = 0 \qquad \text{for } x < a. \tag{25.29}$$

(ii) For $x > b$ the exponentials in the integrand will tend to zero as Re $s \to -\infty$, and so we may close L in the left half-plane, as in figure 25.7(a). Again the integral around Γ vanishes for infinite R, and so, by the residue theorem,

$$f(x) = 0 \qquad \text{for } x > b. \tag{25.30}$$

(iii) For $a < x < b$ the two parts of the integrand behave in different ways and have to be treated separately:

$$I_1 - I_2 \equiv \frac{1}{2\pi i}\int_L \frac{e^{(x-a)s}}{s}\,ds - \frac{1}{2\pi i}\int_L \frac{e^{(x-b)s}}{s}\,ds.$$

The integrand of I_1 then vanishes in the far left-hand half-plane, but does now have a (simple) pole at $s = 0$. Closing L in the left half-plane, and using the residue theorem, we obtain

$$I_1 = \text{residue at } s = 0 \text{ of } s^{-1}e^{(x-a)s} = 1. \tag{25.31}$$

The integrand of I_2, however, vanishes in the far right-hand half-plane (and also has a simple pole at $s = 0$) and is evaluated by a circular-arc completion in that half-plane. Such a contour encloses no poles and leads to $I_2 = 0$.

Thus, collecting together results (25.29)–(25.31) we obtain

$$f(x) = \begin{cases} 0 & \text{for } x < a, \\ 1 & \text{for } a < x < b, \\ 0 & \text{for } x > b, \end{cases}$$

as shown in figure 25.8. ◄

25.6 Stokes' equation and Airy integrals

Much of the analysis of situations occurring in physics and engineering is concerned with what happens at a boundary within or surrounding a physical system. Sometimes the existence of a boundary imposes conditions on the behaviour of variables describing the state of the system; obvious examples include the zero displacement at its end-points of an anchored vibrating string and the zero potential contour that must coincide with a grounded electrical conductor.

More subtle are the effects at internal boundaries, where the same non-vanishing variable has to describe the situation on either side of the boundary but its behaviour is quantitatively, or even *qualitatively*, different in the two regions. In this section we will study an equation, Stokes' equation, whose solutions have this latter property; as well as solutions written as series in the usual way, we will find others expressed as complex integrals.

The Stokes' equation can be written in several forms, e.g.

$$\frac{d^2y}{dx^2} + \lambda xy = 0; \quad \frac{d^2y}{dx^2} + xy = 0; \quad \frac{d^2y}{dx^2} = xy.$$

We will adopt the last of these, but write it as

$$\frac{d^2y}{dz^2} = zy \tag{25.32}$$

to emphasis that its complex solutions are valid for a complex independent variable z, though this also means that particular care has to be exercised when examining their behaviour in different parts of the complex z-plane. The other forms of Stokes' equation can all be reduced to that of (25.32) by suitable (complex) scaling of the independent variable.

25.6.1 The solutions of Stokes' equation

It will be immediately apparent that, even for z restricted to be real and denoted by x, the behaviour of the solutions to (25.32) will change markedly as x passes through $x = 0$. For positive x they will have similar characteristics to the solutions of $y'' = k^2y$, where k is real; these have monotonic exponential forms, either increasing or decreasing. On the other hand, when x is negative the solutions will be similar to those of $y'' + k^2y = 0$, i.e. oscillatory functions of x. This is just the sort of behaviour shown by the wavefunction describing light diffracted by a sharp edge or by the quantum wavefunction describing a particle near to the boundary of a region which it is classically forbidden to enter on energy grounds. Other examples could be taken from the propagation of electromagnetic radiation in an ion plasma or wave-guide.

Let us examine in a bit more detail the behaviour of plots of possible solutions $y(z)$ of Stokes' equation in the region near $z = 0$ and, in particular, what may

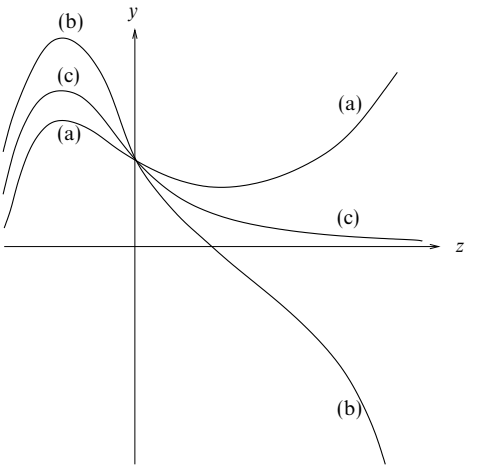


Figure 25.9 Behaviour of the solutions $y(z)$ of Stokes' equation near $z = 0$ for various values of $\lambda = -y'(0)$. (a) with λ small, (b) with λ large and (c) with λ appropriate to the Airy function $\mathrm{Ai}(z)$.

happen in the region $z > 0$. For definiteness and ease of illustration (see figure 25.9), let us suppose that both y and z, and hence the derivatives of y, are real and that $y(0)$ is positive; if it were negative, our conclusions would not be changed since equation (25.32) is invariant under $y(z) \to -y(z)$. The only difference would be that all plots of $y(z)$ would be reflected in the z-axis.

We first note that d^2y/dx^2, and hence also the curvature of the plot, has the same sign as z, i.e. it has positive curvature when $z > 0$, for so long as $y(z)$ remains positive there. What will happen to the plot for $z > 0$ therefore depends crucially on the value of $y'(0)$. If this slope is positive or only slightly negative the positive curvature will carry the plot, either immediately or ultimately, further away from the z-axis. On the other hand, if $y'(0)$ is negative but sufficiently large in magnitude, the plot will cross the $y = 0$ line; if this happens the sign of the curvature reverses and again the plot will be carried ever further from the z-axis, only this time towards large negative values.

Between these two extremes it seems at least plausible that there is a particular negative value of $y'(0)$ that leads to a plot that approaches the z-axis asymptotically, never crosses it (and so always has positive curvature), and has a slope that, whilst always negative, tends to zero in magnitude. There is such a solution, known as $\mathrm{Ai}(z)$, whose properties we will examine further in the following subsections. The three cases are illustrated in figure 25.9.

The behaviour of the solutions of (25.32) in the region $z < 0$ is more straight-

forward, in that, whatever the sign of y at any particular point z, the curvature always has the opposite sign. Consequently the curve always bends towards the z-axis, crosses it, and then bends towards the axis again. Thus the curve exhibits oscillatory behaviour. Furthermore, as $-z$ increases, the curvature for any given $|y|$ gets larger; as a consequence, the oscillations become increasingly more rapid and their amplitude decreases.

25.6.2 Series solution of Stokes' equation

Obtaining a series solution of Stokes' equation presents no particular difficulty when the methods of chapter 16 are used. The equation, written in the form

$$\frac{d^2y}{dz^2} - zy = 0,$$

has no singular points except at $z = \infty$. Every other point in the z-plane is an ordinary point and so two linearly independent series expansions about it (formally with indicial values $\sigma = 0$ and $\sigma = 1$) can be found. Those about $z = 0$ take the forms $\sum_0^\infty a_n z^n$ and $\sum_0^\infty b_n z^{n+1}$. The corresponding recurrence relations are

$$(n+3)(n+2)a_{n+3} = a_n \quad \text{and} \quad (n+4)(n+3)b_{n+3} = b_n,$$

and the two series (with $a_0 = b_0 = 1$) take the forms

$$y_1(z) = 1 + \frac{z^3}{(3)(2)} + \frac{z^6}{(6)(5)(3)(2)} + \cdots,$$
$$y_2(z) = z + \frac{z^4}{(4)(3)} + \frac{z^7}{(7)(6)(4)(3)} + \cdots.$$

The ratios of successive terms for the two series are thus

$$\frac{a_{n+3}z^{n+3}}{a_n z^n} = \frac{z^3}{(n+3)(n+2)} \quad \text{and} \quad \frac{b_{n+3}z^{n+4}}{b_n z^{n+1}} = \frac{z^3}{(n+4)(n+3)}.$$

It follows from the ratio test that both series are absolutely convergent for all z. A similar argument shows that the series for their derivatives are also absolutely convergent for all z. Any solution of the Stokes' equation is representable as a superposition of the two series and so is analytic for all finite z; it is therefore an integral function with its only singularity at infinity.

25.6.3 Contour integral solutions

We now move on to another form of solution of the Stokes' equation (25.32), one that takes the form of a contour integral in which z appears as a parameter in

the integrand. Consider the contour integral

$$y(z) = \int_a^b f(t)\,\exp(zt)\,dt, \tag{25.33}$$

in which a, b and $f(t)$ are all yet to be chosen. Note that the contour is in the complex t-plane and that the path from a to b can be distorted as required so long as no poles of the integrand are trapped between an original path and its distortion.

Substitution of (25.33) into (25.32) yields

$$\begin{aligned}\int_a^b t^2 f(t)\,\exp(zt)\,dt &= \int_a^b z\,f(t)\,\exp(zt)\,dt \\ &= [f(t)\,\exp(zt)]_a^b - \int_a^b \frac{df(t)}{dt}\,\exp(zt)\,dt.\end{aligned}$$

If we could choose the limits a and b so that the end-point contributions vanish then Stokes' equation would be satisfied by (25.33), provided $f(t)$ satisfies

$$\frac{df(t)}{dt} + t^2 f(t) = 0 \quad \Rightarrow \quad f(t) = A\exp(-\tfrac{1}{3}t^3), \tag{25.34}$$

where A is any constant.

To make the end-point contributions vanish we must choose a and b such that $\exp(-\frac{1}{3}t^3 + zt) = 0$ for both values of t. This can only happen if $|a| \to \infty$ and $|b| \to \infty$ and, even then, only if Re (t^3) is positive. This condition is satisfied if

$$2n\pi - \tfrac{1}{2}\pi < 3\arg(t) < 2n\pi + \tfrac{1}{2}\pi \text{ for some integer } n.$$

Thus a and b must each be at infinity in one of the three shaded areas shown in figure 25.10, but clearly not in the same area as this would lead to a zero value for the contour integral. This leaves three contours (marked C_1, C_2 and C_3 in the figure) that start and end in different sectors. However, only two of them give rise to independent integrals since the path $C_2 + C_3$ is equivalent to (can be distorted into) the path C_1.

The two integral functions given particular names are

$$\mathrm{Ai}(z) = \frac{1}{2\pi i}\int_{C_1} \exp(-\tfrac{1}{3}t^3 + zt)\,dt \tag{25.35}$$

and

$$\mathrm{Bi}(z) = \frac{1}{2\pi}\int_{C_2} \exp(-\tfrac{1}{3}t^3 + zt)\,dt - \frac{1}{2\pi}\int_{C_3} \exp(-\tfrac{1}{3}t^3 + zt)\,dt. \tag{25.36}$$

Stokes' equation is unchanged if the independent variable is changed from z to ζ, where $\zeta = \exp(2\pi i/3)z \equiv \Omega z$. This is also true for the repeated change $z \to \Omega\zeta = \Omega^2 z$. The same changes of variable, rotations of the complex plane through $2\pi/3$ or $4\pi/3$, carry the three contours C_1, C_2 and C_3 into each other,

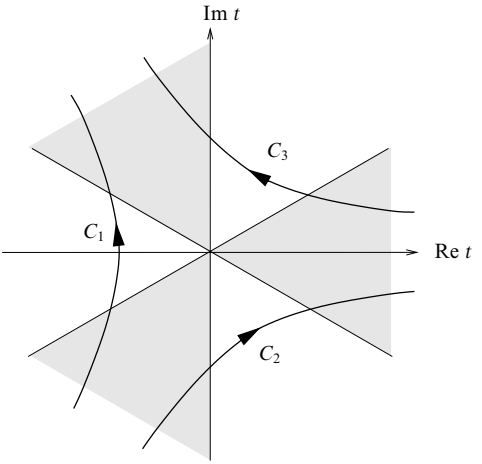


Figure 25.10 The contours used in the complex t-plane to define the functions $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$.

though sometimes the sense of traversal is reversed. Consequently there are relationships connecting Ai and Bi when the rotated variables are used as their arguments. As two examples,

$$\mathrm{Ai}(z) + \Omega\mathrm{Ai}(\Omega z) + \Omega^2\mathrm{Ai}(\Omega^2 z) = 0, \tag{25.37}$$

$$\mathrm{Bi}(z) = i[\,\Omega^2\mathrm{Ai}(\Omega^2 z) - \Omega\mathrm{Ai}(\Omega z)\,] = e^{-\pi i/6}\mathrm{Ai}(ze^{-2\pi i/3}) + e^{\pi i/6}\mathrm{Ai}(ze^{2\pi i/3}). \tag{25.38}$$

Since the only requirements for the integral paths is that they start and end in the correct sectors, we can distort path C_1 so that it lies on the imaginary axis for virtually its whole length and just to the left of the axis at its two ends. This enables us to obtain an alternative expression for $\mathrm{Ai}(z)$, as follows.

Setting $t = is$, where s is real and $-\infty < s < \infty$, converts the integral representation of $\mathrm{Ai}(z)$ to

$$\mathrm{Ai}(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp[\,i(\tfrac{1}{3}s^3 + zs)\,]\,ds.$$

Now, the exponent in this integral is an odd function of s and so the imaginary part of the integrand contributes nothing to the integral. What is left is therefore

$$\mathrm{Ai}(z) = \frac{1}{\pi}\int_{0}^{\infty} \cos(\tfrac{1}{3}s^3 + zs)\,ds. \tag{25.39}$$

This form shows explicitly that when z is real, so is $\mathrm{Ai}(z)$.

This same representation can also be used to justify the association of the

contour integral (25.35) with the particular solution of Stokes' equation that decays monotonically to zero for real $z > 0$ as $|z| \to \infty$. As discussed in subsection 25.6.1, all solutions except the one called $\mathrm{Ai}(z)$ tend to $\pm\infty$ as z (real) takes on increasingly large positive values and so their asymptotic forms reflect this. In a worked example in subsection 25.8.2 we use the method of steepest descents (a saddle-point method) to show that the function defined by (25.39) has exactly the characteristic asymptotic property expected of $\mathrm{Ai}(z)$ (see page 911). It follows that it is the same function as $\mathrm{Ai}(z)$, up to a real multiplicative constant.

The choice of definition (25.36) as the other named solution $\mathrm{Bi}(z)$ of Stokes' equation is a less obvious one. However, it is made on the basis of its behaviour for negative real values of z. As discussed earlier, $\mathrm{Ai}(z)$ oscillates almost sinusoidally in this region, except for a relatively slow increase in frequency and an even slower decrease in amplitude as $-z$ increases. The solution $\mathrm{Bi}(z)$ is chosen to be the particular function that exhibits the same behaviour as $\mathrm{Ai}(z)$ except that it is in quadrature with Ai, i.e. it is $\pi/2$ out of phase with it. Specifically, as $x \to -\infty$,

$$\mathrm{Ai}(x) \sim \frac{1}{\sqrt{2\pi}x^{1/4}} \sin\left(\frac{2|x|^{3/2}}{3} + \frac{\pi}{4}\right), \tag{25.40}$$

$$\mathrm{Bi}(x) \sim \frac{1}{\sqrt{2\pi}x^{1/4}} \cos\left(\frac{2|x|^{3/2}}{3} + \frac{\pi}{4}\right). \tag{25.41}$$

There is a close parallel between this choice and that of taking sine and cosine functions as the basic independent solutions of the simple harmonic oscillator equation. Plots of $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$ for real z are shown in figure 25.11.

►*By choosing a suitable contour for C_1 in (25.35), express* $\mathrm{Ai}(0)$ *in terms of the gamma function.*

With z set equal to zero, (25.35) takes the form

$$\mathrm{Ai}(0) = \frac{1}{2\pi i} \int_{C_1} \exp(-\tfrac{1}{3}t^3)\, dt.$$

We again use the freedom to choose the specific line of the contour so as to make the actual integration as simple as possible.

Here we consider C_1 as made up of two straight-line segments: one along the line $\arg t = 4\pi/3$, starting at infinity in the correct sector and ending at the origin; the other starting at the origin and going to infinity along the line $\arg t = 2\pi/3$, thus ending in the correct final sector. On each, we set $\frac{1}{3}t^3 = s$, where s is real and positive on both lines. Then $dt = e^{4\pi i/3}(3s)^{-2/3}\, ds$ on the first segment and $dt = e^{2\pi i/3}(3s)^{-2/3}\, ds$ on the second.

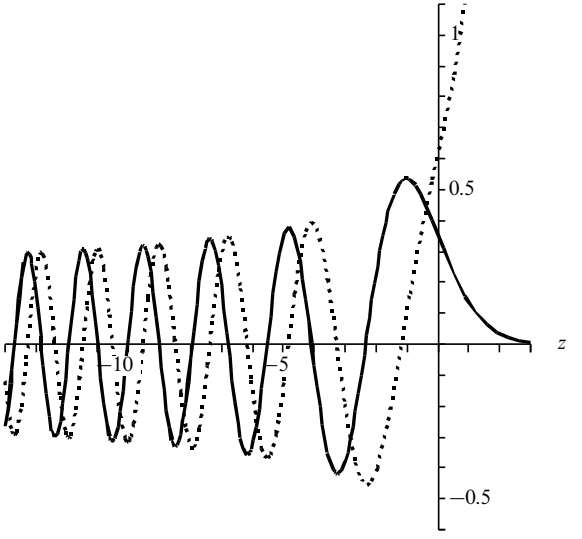


Figure 25.11 The functions Ai(z) (full line) and Bi(z) (broken line) for real z.

Then we have

$$\begin{aligned}\mathrm{Ai}(0) &= \frac{1}{2\pi i}\int_{\infty}^{0} e^{-s}e^{4\pi i/3}(3s)^{-2/3}\,ds + \frac{1}{2\pi i}\int_{0}^{\infty} e^{-s}e^{2\pi i/3}(3s)^{-2/3}\,ds \\ &= \frac{3^{-2/3}}{2\pi i}\int_{0}^{\infty} e^{-s}(-e^{4\pi i/3}+e^{2\pi i/3})s^{-2/3}\,ds \\ &= \frac{\sqrt{3}i\,3^{-2/3}}{2\pi i}\int_{0}^{\infty} e^{-s}s^{-2/3}\,ds \\ &= \frac{3^{-1/6}}{2\pi}\Gamma(\tfrac{1}{3}),\end{aligned}$$

where we have used the standard integral defining the gamma function in the last line. ◄

Finally in this subsection we should mention that the Airy functions and their derivatives are closely related to Bessel functions of orders $\pm\frac{1}{3}$ and $\pm\frac{2}{3}$ and that

there exist many representations, both as linear combinations and as indefinite integrals, of one in terms of the other.§

25.7 WKB methods

Throughout this book we have had many occasions on which it has been necessary to solve the equation

$$\frac{d^2y}{dx^2} + k_0^2 f(x) y = 0 \tag{25.42}$$

when the notionally general function $f(x)$ has been, in fact, a constant, usually the unit function $f(x) = 1$. Then the solutions have been elementary and of the form $A \sin k_0 x$ or $A \cos k_0 x$ with arbitrary but constant amplitude A.

Explicit solutions of (25.42) for a non-constant $f(x)$ are only possible in a limited number of cases, but, as we will show, some progress can be made if $f(x)$ is a slowly varying function of x, in the sense that it does not change much in a range of x of the order of k_0^{-1}.

We will also see that it is possible to handle situations in which $f(x)$ is complex; this enables us to deal with, for example, the passage of waves through an absorbing medium. Developing such solutions will involve us in finding the integrals of some complex quantities, integrals that will behave differently in the various parts of the complex plane – hence their inclusion in this chapter.

25.7.1 Phase memory

Before moving on to the formal development of WKB methods¶ we discuss the concept of *phase memory* which is the underlying idea behind them.

Let us first suppose that $f(x)$ is real, positive and essentially constant over a range of x and define $n(x)$ as the positive square root of $f(x)$; $n(x)$ is then also real, positive and essentially constant over the same range of x. We adopt this notation so that the connection can be made with the description of an electromagnetic wave travelling through a medium of dielectric constant $f(x)$ and, consequently, refractive index $n(x)$. The quantity $y(x)$ would be the electric or magnetic field of the wave. For this simplified case, in which we can omit the

§ These relationships and many other properties of the Airy functions can be found in, for example, M. Abramowitz and I. A. Stegun (eds), *Handbook of Mathematical Functions* (New York: Dover, 1965) pp. 446–50.

¶ So called because they were used, independently, by Wentzel, Kramers and Brillouin to tackle certain wave-mechanical problems in 1926, though they had earlier been studied in some depth by Jeffreys and used as far back as the first half of the nineteenth century by Green.

x-dependence of $n(x)$, the solution would be (as usual)

$$y(x) = A\exp(-ik_0 nx), \tag{25.43}$$

with both A and n constant. The quantity $k_0 nx$ would be real and would be called the 'phase' of the wave; it increases linearly with x.

As a first variation on this simple picture, we may allow $f(x)$ to be complex, though, for the moment, still constant. Then $n(x)$ is still a constant, albeit a complex one:

$$n = \mu + iv.$$

The solution is formally the same as before; however, whilst it still exhibits oscillatory behaviour, the amplitude of the oscillations either grows or declines, depending upon the sign of v:

$$y(x) = A\exp(-ik_0 nx) = A\exp[-ik_0(\mu + iv)x] = A\exp(k_0 vx)\exp(-ik_0 \mu x).$$

This solution with v negative is the appropriate description for a wave travelling in a uniform absorbing medium. The quantity $k_0(\mu + iv)x$ is usually called the *complex phase* of the wave.

We now allow $f(x)$, and hence $n(x)$, to be both complex and varying with position, though, as we have noted earlier, there will be restrictions on how rapidly $f(x)$ may vary if valid solutions are to be obtained. The obvious extension of solution (25.43) to the present case would be

$$y(x) = A\exp[-ik_0 n(x)x], \tag{25.44}$$

but direct substitution of this into equation (25.42) gives

$$y'' + k_0^2 n^2 y = -k_0^2(n'^2 x^2 + 2nn'x)y - ik_0(n''x + 2n')y.$$

Clearly the RHS can only be zero, as is required by the equation, if n' and n'' are both very small, or if some unlikely relationship exists between them.

To try to improve on this situation, we consider how the phase ϕ of the solution changes as the wave passes through an infinitesimal thickness dx of the medium. The infinitesimal (complex) phase change $d\phi$ for this is clearly $k_0 n(x)\,dx$, and therefore will be

$$\Delta\phi = k_0 \int_0^x n(u)\,du$$

for a finite thickness x of the medium. This suggests that an improvement on (25.44) might be

$$y(x) = A\exp\left(-ik_0 \int_0^x n(u)\,du\right). \tag{25.45}$$

This is still not an exact solution as now

$$y''(x) + k_0^2 n^2(x)y(x) = -ik_0 n'(x)y(x).$$

This still requires $k_0 n'(x)$ to be small (compared with, say, $k_0^2 n^2(x)$), but is some improvement (not least in complexity!) on (25.44) and gives some measure of the conditions under which the solution might be a suitable approximation.

The integral in equation (25.45) embodies what is sometimes referred to as the *phase memory* approach; it expresses the notion that the phase of the wave-like solution is the cumulative effect of changes it undergoes as it passes through the medium. If the medium were uniform the overall change would be proportional to nx, as in (25.43); the extent to which it is not uniform is reflected in the amount by which the integral differs from nx.

The condition for solution (25.45) to be a reasonable approximation can be written as $n' k_0^{-1} \ll n^2$ or, in words, the change in n over an x-range of k_0^{-1} should be small compared with n^2. For light in an optical medium, this means that the refractive index n, which is of the order of unity, must change very little over a distance of a few wavelengths.

For some purposes the above approximation is adequate, but for others further refinement is needed. This comes from considering solutions that are still wave-like but have amplitudes, as well as phases, that vary with position. These are the WKB solutions developed and studied in the next three subsections.

25.7.2 Constructing the WKB solutions

Having formulated the notion of phase memory, we now construct the WKB solutions of the general equation (25.42), in which $f(x)$ can now be both position-dependent and complex. As we have already seen, it is the possibility of a complex phase that permits the existence of wave-like solutions with varying amplitudes. Since $n(x)$ is calculated as the square root of $f(x)$, there is an ambiguity in its overall sign. In physical applications this is normally resolved unambiguously by considerations such as the inevitable increase in entropy of the system, but, so far as dealing with purely mathematical questions is concerned, the ambiguity must be borne in mind.

The process we adopt is an iterative one based on the assumption that the second derivative of the complex phase with respect to x is very small and can be approximated at each stage of the iteration. So we start with equation (25.42) and look for a solution of the form

$$y(x) = A \exp[\, i\phi(x)\,], \tag{25.46}$$

where A is a constant. When this is substituted into (25.42) the equation becomes

$$\left[-\left(\frac{d\phi}{dx}\right)^2 + i\frac{d^2\phi}{dx^2} + k_0^2 n^2(x) \right] y(x) = 0. \tag{25.47}$$

Setting the quantity in square brackets to zero produces a non-linear equation for

which there is no obvious solution for a general $n(x)$. However, on the assumption that $d^2\phi/dx^2$ is small, an iterative solution can be found.

As a first approximation ϕ'' is ignored, and the solution

$$\frac{d\phi}{dx} \approx \pm k_0 n(x)$$

is obtained. From this, differentiation gives an approximate value for

$$\frac{d^2\phi}{dx^2} \approx \pm k_0 \frac{dn}{dx},$$

which can be substituted into equation (25.47) to give, as a second approximation for $d\phi/dx$, the expression

$$\begin{aligned}\frac{d\phi}{dx} &\approx \pm \left[k_0^2 n^2(x) \pm i k_0 \frac{dn}{dx} \right]^{1/2} \\ &= \pm k_0 n \left(1 \pm \frac{i}{2k_0 n^2} \frac{dn}{dx} + \cdots \right) \\ &\approx \pm k_0 n + \frac{i}{2n} \frac{dn}{dx}.\end{aligned}$$

This can now be integrated to give an approximate expression for $\phi(x)$ as follows:

$$\phi(x) = \pm k_0 \int_{x_0}^{x} n(u)\, du + \frac{i}{2} \ln[\, n(x)\,], \tag{25.48}$$

where the constant of integration has been formally incorporated into the lower limit x_0 of the integral. Now, noting that $\exp(i\,\frac{1}{2}i \ln n) = n^{-1/2}$, substitution of (25.48) into equation (25.46) gives

$$y_{\pm}(x) = \frac{A}{n^{1/2}} \exp\left[\pm i k_0 \int_{x_0}^{x} n(u)\, du \right] \tag{25.49}$$

as two independent WKB solutions of the original equation (25.42). This result is essentially the same as that in (25.45) except that the amplitude has been divided by $\sqrt{n(x)}$, i.e. by $[\, f(x)\,]^{1/4}$. Since $f(x)$ may be complex, this may introduce an additional x-dependent phase into the solution as well as the more obvious change in amplitude.

► *Find two independent WKB solutions of Stokes' equation in the form*

$$\frac{d^2y}{dx^2} + \lambda x y = 0, \textit{ with } \lambda \textit{ real and} > 0.$$

The form of the equation is the same as that in (25.42) with $f(x) = x$, and therefore $n(x) = x^{1/2}$. The WKB solutions can be read off immediately using (25.49), so long as we remember that although $f(x)$ is real, it has four fourth roots and that therefore the constant appearing in a solution can be complex. Two independent WKB solutions are

$$y_{\pm}(x) = \frac{A_{\pm}}{|x|^{1/4}} \exp\left[\pm i\sqrt{\lambda} \int^{x} \sqrt{u}\, du \right] = \frac{A_{\pm}}{|x|^{1/4}} \exp\left[\pm i \frac{2\sqrt{\lambda}}{3} x^{3/2} \right]. \tag{25.50}$$

The precise combination of these two solutions that is required for any particular problem has to be determined from the problem. ◄

When Stokes' equation is applied more generally to functions of a complex variable, i.e. the real variable x is replaced by the complex variable z, it has solutions whose type of behaviour depends upon where z lies in the complex plane. For the particular case $\lambda = -1$, when Stokes' equation takes the form

$$\frac{d^2y}{dz^2} = zy$$

and the two WKB solutions (with the inverse fourth root written explicitly) are

$$y_{1,2}(z) = \frac{A_{1,2}}{z^{1/4}} \exp\left[\mp\frac{2}{3}z^{3/2}\right], \tag{25.51}$$

one of the solutions, $\mathrm{Ai}(z)$ (see section 25.6), has the property that it is real whenever z is real, whether positive or negative. For negative real z it has sinusoidal behaviour, but it becomes an evanescent wave for real positive z.

Since the function $z^{3/2}$ has a branch point at $z = 0$ and therefore has an abrupt (complex) change in its argument there, it is clear that neither of the two functions in (25.51), nor any fixed combination of them, can be equal to $\mathrm{Ai}(z)$ for all values of z. More explicitly, for z real and positive, $\mathrm{Ai}(z)$ is proportional to $y_1(z)$, which is real and has the form of a decaying exponential function, whilst for z real and negative, when $z^{3/2}$ is purely imaginary and $y_1(z)$ and $y_2(z)$ are both oscillatory, it is clear that $\mathrm{Ai}(z)$ must contain both y_1 and y_2 with equal amplitudes.

The actual combinations of $y_1(z)$ and $y_2(z)$ needed to coincide with these two asymptotic forms of $\mathrm{Ai}(z)$ are as follows.

For z real and > 0,
$$c_1 y_1(z) = \frac{1}{2\sqrt{\pi}z^{1/4}} \exp\left[-\frac{2}{3}z^{3/2}\right]. \tag{25.52}$$

For z real and < 0,
$$c_2[\,y_1(z)e^{i\pi/4} - y_2(z)e^{-i\pi/4}\,] = \frac{1}{\sqrt{\pi}(-z)^{1/4}} \sin\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right]. \tag{25.53}$$

Therefore it must be the case that the constants used to form $\mathrm{Ai}(z)$ from the solutions (25.51) change as z moves from one part of the complex plane to another. In fact, the changes occur for particular values of the argument of z; these boundaries are therefore radial lines in the complex plane and are known as *Stokes lines*. For Stokes' equation they occur when $\arg z$ is equal to 0, $2\pi/3$ or $4\pi/3$.

The general occurrence of a change in the arbitrary constants used to make up a solution, as its argument crosses certain boundaries in the complex plane, is known as the Stokes phenomenon and is discussed further in subsection 25.7.4.

►*Apply the WKB method to the problem of finding the quantum energy levels E of a particle of mass m bound in a symmetrical one-dimensional potential well V(x) that has only a single minimum. The relevant Schrödinger equation is*

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi.$$

Relate the problem close to each of the classical 'turning points', $x = \pm a$ at which $E - V(x) = 0$, to Stokes' equation and assume that it is appropriate to use the solution Ai(x) *given in equations (25.52) and (25.53) at $x = a$. Show that if the general WKB solution in the 'classically allowed' region $-a < x < a$ is to match such Airy solutions at* both *turning points, then*

$$\int_{-a}^{a} k(x)\,dx = (n + \tfrac{1}{2})\pi,$$

where $k^2(x) = 2m[E - V(x)]/\hbar^2$ and $n = 0, 1, 2, \ldots$.

For a symmetric potential $V(x) = V_0 x^{2s}$, where s is a positive integer, show that in this approximation the energy of the nth level is given by $E_n = c_s(n + \frac{1}{2})^{2s/(s+1)}$, where c_s is a constant depending on s but not upon n.

We start by multiplying the equation through by $2m/\hbar^2$, writing $2m[E - V(x)]/\hbar^2$ as $k^2(x)$, and rearranging the equation to read

$$\frac{d^2\psi}{dx^2} + k^2(x)\psi = 0, \tag{25.54}$$

noting that, with E and $V(x)$ given, the equation $E = V(a)$ determines the value of a and that $k(a) = 0$.

For $-a < x < a$, where $k^2(x)$ is positive, the form of the WKB solutions are given directly by (25.49) as

$$\psi_{\pm} = \frac{C}{\sqrt{k(x)}} \exp\left[\pm i \int^{x} k(u)\,du\right].$$

Just beyond the turning point $x = a$, where

$$E - V(x) = 0 - V'(a)(x - a) + \mathrm{O}[(x - a)^2],$$

equation (25.54) can be approximated by

$$\frac{d^2\psi}{dx^2} - \frac{2mV'(a)}{\hbar^2}(x - a)\psi = 0. \tag{25.55}$$

This, in turn, can be reduced to Stokes' equation by first setting $x - a = \mu z$ and $\psi(x) \equiv y(z)$, so converting it into

$$\frac{1}{\mu^2}\frac{d^2y}{dz^2} - \frac{2\mu mV'(a)}{\hbar^2} zy = 0,$$

and then choosing $\mu = [\hbar^2/2mV'(a)]^{1/3}$. The equation then reads

$$\frac{d^2y}{dz^2} = zy.$$

Since the solution must be evanescent for $x > a$, i.e. for $z > 0$, we assume that the appropriate solution there is Ai(z); this implies that, for z small and negative (just inside the classically allowed region), the solution has the form given by (25.53), namely

$$\frac{A}{(-z)^{1/4}} \sin\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right],$$

for some constant A. This form is only valid for negative z close to $z = 0$ and is not appropriate within the well as a whole, where the approximation (25.55) leading to Stokes' equation is not valid. However, it does allow us to determine the correct combination of the WKB solutions found earlier for the proper continuation inside the well of the solution found for $z > 0$. This is

$$\psi_1(x) = \frac{A}{\sqrt{k(x)}} \sin\left(\int_x^a k(u)\,du + \frac{\pi}{4}\right).$$

A similar argument gives the continuation inside the well of the evanescent solution required in the region $x < -a$ as

$$\psi_2(x) = \frac{B}{\sqrt{k(x)}} \sin\left(\int_{-a}^x k(u)\,du + \frac{\pi}{4}\right).$$

However, for a consistent solution to the problem, these two functions must match, both in magnitude and slope, at any arbitrary point x inside the well.We therefore require both of the equalities

$$\frac{A}{\sqrt{k(x)}} \sin\left(\int_x^a k(u)\,du + \frac{\pi}{4}\right) = \frac{B}{\sqrt{k(x)}} \sin\left(\int_{-a}^x k(u)\,du + \frac{\pi}{4}\right) \qquad \text{(i)}$$

and

$$-\frac{1}{2}\frac{Ak'}{\sqrt{k^3(x)}} \sin\left(\int_x^a k(u)\,du + \frac{\pi}{4}\right) + \frac{A}{\sqrt{k(x)}}\,[-k(x)] \cos\left(\int_x^a k(u)\,du + \frac{\pi}{4}\right)$$

$$= -\frac{1}{2}\frac{Bk'}{\sqrt{k^3(x)}} \sin\left(\int_{-a}^x k(u)\,du + \frac{\pi}{4}\right) + \frac{B}{\sqrt{k(x)}}\,[k(x)] \cos\left(\int_{-a}^x k(u)\,du + \frac{\pi}{4}\right). \qquad \text{(ii)}$$

The general condition for the validity of the WKB solutions is that the derivatives of the function appearing in the phase integral are small in some sense (see subsection 25.7.3 for a more general discussion); here, if $k'/\sqrt{k^3} \ll k/\sqrt{k}$, i.e. $k' \ll k^2$, then we can ignore the k' terms in equation (ii) above. In fact, for this particular situation, this approximation is not needed since the first of the equalities, equation (i), ensures that the k'-dependent terms in the second equality (ii) cancel. Either way, we are left with a pair of homogeneous equations for A and B. For them to give consistent values for the ratio A/B, it must be that

$$\frac{A}{\sqrt{k(x)}} \sin\left(\int_x^a k(u)\,du + \frac{\pi}{4}\right) \times \frac{B}{\sqrt{k(x)}}\,[k(x)] \cos\left(\int_{-a}^x k(u)\,du + \frac{\pi}{4}\right)$$

$$= \frac{A}{\sqrt{k(x)}}\,[-k(x)] \cos\left(\int_x^a k(u)\,du + \frac{\pi}{4}\right) \times \frac{B}{\sqrt{k(x)}} \sin\left(\int_{-a}^x k(u)\,du + \frac{\pi}{4}\right).$$

This condition reduces to

$$\sin\left[\left(\int_x^a k(u)\,du + \frac{\pi}{4}\right) + \left(\int_{-a}^x k(u)\,du + \frac{\pi}{4}\right)\right] = 0,$$

$$\sin\left[\left(\int_{-a}^a k(u)\,du + \frac{\pi}{2}\right)\right] = 0,$$

$$\Rightarrow \quad \int_{-a}^a k(u)\,du = (n + \tfrac{1}{2})\pi.$$

Since $k(x) > 0$ in the range $-a < x < a$, n may take the values 0, 1, 2, ...

If $V(x)$ has the form $V(x) = V_0 x^{2s}$ then, for the nth allowed energy level, $E_n = V_0 a_n^{2s}$ and

$$k^2(x) = \frac{2m}{\hbar^2}(E_n - V_0 x^{2s}).$$

The result just proved gives

$$\int_{-a_n}^{a_n} \frac{\sqrt{2mV_0}}{\hbar} (a_n^{2s} - x^{2s})^{1/2}\, dx = (n + \tfrac{1}{2})\pi.$$

Writing $x = va_n$ shows that the integral is proportional to $a_n^{s+1} I_s$, where I_s is the integral between -1 and $+1$ of $(1 - v^{2s})^{1/2}$ and does not depend upon n. Thus $E_n \propto a_n^{2s}$ and $a_n^{s+1} \propto (n + \frac{1}{2})$, implying that $E_n \propto (n + \frac{1}{2})^{2s/s+1}$.

Although not asked for, we note that the above result indicates that, for a simple harmonic oscillator, for which $s = 1$, the energy levels $[E_n \sim (n + \frac{1}{2})]$ are equally spaced, whilst for very large s, corresponding to a square well, the energy levels vary as n^2. Both of these results agree with what is found from detailed analyses of the individual cases. ◄

25.7.3 Accuracy of the WKB solutions

We may also ask when we can expect the WKB solutions to the Stokes' equation to be reasonable approximations. Although our final form for the WKB solutions is not exactly that used when the condition $|n' k_0^{-1}| \ll |n^2|$ was derived, it should give the same order of magnitude restriction as a more careful analysis. For the derivation of (25.51), $k_0^2 = -1$, $n(z) = [f(z)]^{1/2} = z^{1/2}$, and the criterion becomes $\frac{1}{2}|z^{-1/2}| \ll |z|$, or, in round terms, $|z|^3 \gg 1$.

For the more general equation, typified by (25.42), the condition for the validity of the WKB solutions can usually be satisfied by making some quantity, often $|z|$, sufficiently large. Alternatively, a parameter such as k_0 can be made large enough that the validity criterion is satisfied to any pre-specified level. However, from a practical point of view, natural physical parameters cannot be varied at will, and requiring z to be large may well reduce the value of the method to virtually zero. It is normally more useful to try to obtain an improvement on a WKB solution by multiplying it by a series whose terms contain increasing inverse powers of the variable, so that the result can be applied successfully for moderate, and not just excessively large, values of the variable.

We do not have the space to discuss the properties and pitfalls of such asymptotic expansions in any detail, but exercise 25.18 will provide the reader with a model of the general procedure. A few particular points that should be noted are given as follows.

(i) If the multiplier is analytic as $z \to \infty$, then it will be represented by a series that is convergent for $|z|$ greater than some radius of convergence R.

(ii) If the multiplier is not analytic as $z \to \infty$, as is usually the case, then the multiplier series eventually diverges and there is a z-dependent optimal number of terms that the series should contain in order to give the best accuracy.

(iii) For a fixed value of $\arg z$, the asymptotic expansion of the multiplier is unique. However, the same asymptotic expansion can represent more than

one function and the same function may need different expansions for different values of $\arg z$.

Finally in this subsection we note that, although the form of equation (25.42) may appear rather restrictive, in that it contains no term in y', the results obtained so far can be applied to an equation such as

$$\frac{d^2y}{dz^2} + P(z)\frac{dy}{dz} + Q(z)y = 0. \tag{25.56}$$

To make this possible, a change of either the dependent or the independent variable is made. For the former we write

$$Y(z) = y(z)\exp\left(\frac{1}{2}\int^z P(u)\,du\right) \quad \Rightarrow \quad \frac{d^2Y}{dz^2} + \left(Q - \frac{1}{4}P^2 - \frac{1}{2}\frac{dP}{dz}\right)Y = 0,$$

whilst for the latter we introduce a new independent variable ζ defined by

$$\frac{d\zeta}{dz} = \exp\left(-\int^z P(u)\,du\right) \quad \Rightarrow \quad \frac{d^2y}{d\zeta^2} + Q\left(\frac{dz}{d\zeta}\right)^2 y = 0.$$

In either case, equation (25.56) is reduced to the form of (25.42), though it will be clear that the two sets of WKB solutions (which are, of course, only approximations) will not be the same.

25.7.4 The Stokes phenomenon

As we saw in subsection 25.7.2, the combination of WKB solutions of a differential equation required to reproduce the asymptotic form of the accurate solution $y(z)$ of the same equation, varies according to the region of the z-plane in which z lies. We now consider this behaviour, known as the Stokes phenomenon, in a little more detail.

Let $y_1(z)$ and $y_2(z)$ be the two WKB solutions of a second-order differential equation. Then any solution $Y(z)$ of the same equation can be written asymptotically as

$$Y(z) \sim A_1y_1(z) + A_2y_2(z), \tag{25.57}$$

where, although we will be considering (abrupt) changes in them, we will continue to refer to A_1 and A_2 as constants, as they are within any one region. In order to produce the required change in the linear combination, as we pass over a Stokes line from one region of the z-plane to another, one of the constants must change (relative to the other) as the border between the regions is crossed.

At first sight, this may seem impossible without causing a discernible discontinuity in the representation of $Y(z)$. However, we must recall that the WKB solutions are approximations, and that, as they contain a phase integral, for certain values of $\arg z$ the phase $\phi(z)$ will be purely imaginary and the factors

$\exp[\pm i\phi(z)]$ will be purely real. What is more, one such factor, known as the *dominant* term, will be exponentially large, whilst the other (the *subdominant* term) will be exponentially small. A *Stokes line* is precisely where this happens.

We can now see how the change takes place without an observable discontinuity occurring. Suppose that $y_1(z)$ is very large and $y_2(z)$ is very small on a Stokes line. Then a finite change in A_2 will have a negligible effect on $Y(z)$; in fact, Stokes showed, for some particular cases, that the change is less than the uncertainty in $y_1(z)$ arising from the approximations made in deriving it. Since the solution with any particular asymptotic form is determined in a region bounded by two Stokes lines to within an overall multiplicative constant and the original equation is linear, the change in A_2 when one of the Stokes lines is crossed must be proportional to A_1, i.e. A_2 changes to $A_2 + SA_1$, where S is a constant (the *Stokes constant*) characteristic of the particular line but independent of A_1 and A_2. It should be emphasised that, at a Stokes line, if the dominant term is not present in a solution, then the multiplicative constant in the subdominant term *cannot* change as the line is crossed.

As an example, consider the Bessel function $J_0(z)$ of zero order. It is single-valued, differentiable everywhere, and can be written as a series in powers of z^2. It is therefore an integral even function of z. However, its asymptotic approximations for two regions of the z-plane, $\mathrm{Re}\, z > 0$ and z real and negative, are given by

$$J_0(z) \sim \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{z}}\left(e^{iz}e^{-i\pi/4} + e^{-iz}e^{i\pi/4}\right), \quad |\arg(z)| < \tfrac{1}{2}\pi,\ |\arg(z^{-1/2})| < \tfrac{1}{4}\pi,$$

$$J_0(z) \sim \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{z}}\left(e^{iz}e^{3i\pi/4} + e^{-iz}e^{i\pi/4}\right), \quad \arg(z) = \pi,\ \arg(z^{-1/2}) = -\tfrac{1}{2}\pi.$$

We note in passing that neither of these expressions is naturally single-valued, and a prescription for taking the square root has to be given. Equally, neither is an even function of z. For our present purpose the important point to note is that, for both expressions, on the line $\arg z = \pi/2$ both z-dependent exponents become real. For large $|z|$ the second term in each expression is large; this is the dominant term, and its multiplying constant $e^{i\pi/4}$ is the same in both expressions. Contrarywise, the first term in each expression is small, and its multiplying constant does change, from $e^{-i\pi/4}$ to $e^{3i\pi/4}$, as $\arg z$ passes through $\pi/2$ whilst increasing from 0 to π. It is straightforward to calculate the Stokes constant for this Stokes line as follows:

$$S = \frac{A_2(\text{new}) - A_2(\text{old})}{A_1} = \frac{e^{3i\pi/4} - e^{-i\pi/4}}{e^{i\pi/4}} = e^{i\pi/2} - e^{-i\pi/2} = 2i.$$

If we had moved (in the negative sense) from $\arg z = 0$ to $\arg z = -\pi$, the relevant Stokes line would have been $\arg z = -\pi/2$. There the first term in each expression is dominant, and it would have been the constant $e^{i\pi/4}$ in the second term that would have changed. The final argument of $z^{-1/2}$ would have been $+\pi/2$.

Finally, we should mention that the lines in the z-plane on which the exponents in the WKB solutions are purely imaginary, and the two solutions have equal amplitudes, are usually called the *anti-Stokes lines*. For the general Bessel's equation they are the real positive and real negative axes.

25.8 Approximations to integrals

In this section we will investigate a method of finding approximations to the values or forms of certain types of infinite integrals. The class of integrals to be considered is that containing integrands that are, or can be, represented by exponential functions of the general form $g(z)\exp[f(z)]$. The exponents $f(z)$ may be complex, and so integrals of sinusoids can be handled as well as those with more obvious exponential properties. We will be using the analyticity properties of the functions of a complex variable to move the integration path to a part of the complex plane where a general integrand can be approximated well by a standard form; the standard form is then integrated explicitly.

The particular standard form to be employed is that of a Gausssian function of a real variable, for which the integral between infinite limits is well known. This form will be generated by expressing $f(z)$ as a Taylor series expansion about a point z_0, at which the linear term in the expansion vanishes, i.e. where $f'(z) = 0$. Then, apart from a constant multiplier, the exponential function will behave like $\exp[\frac{1}{2}f''(z_0)(z - z_0)^2]$ and, by choosing an appropriate direction for the contour to take as it passes through the point, this can be made into a normal Gaussian function of a real variable and its integral may then be found.

25.8.1 Level lines and saddle points

Before we can discuss the method outlined above in more detail, a number of observations about functions of a complex variable and, in particular, about the properties of the exponential function need to be made. For a general analytic function,

$$f(z) = \phi(x, y) + i\psi(x, y), \tag{25.58}$$

of the complex variable $z = x + iy$, we recall that, not only do both ϕ and ψ satisfy Laplace's equation, but $\nabla\phi$ and $\nabla\psi$ are orthogonal. This means that the lines on which one of ϕ and ψ is constant are exactly the lines on which the other is changing most rapidly.

Let us apply these observations to the function

$$h(z) \equiv \exp[f(z)] = \exp(\phi)\exp(i\psi), \tag{25.59}$$

recalling that the functions ϕ and ψ are themselves real. The magnitude of $h(z)$, given by $\exp(\phi)$, is constant on the lines of constant ϕ, which are known as the

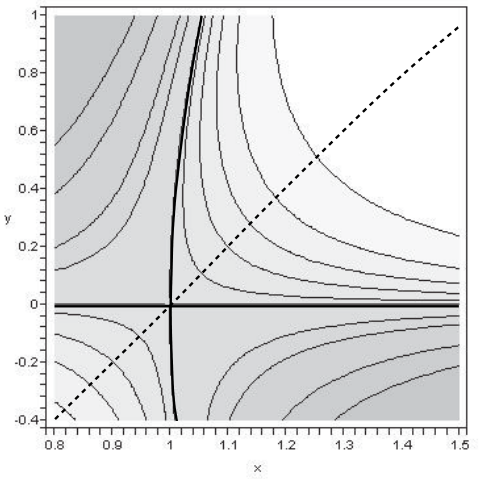


Figure 25.12 A greyscale plot with associated contours of the value of $|h(z)|$, where $h(z) = \exp[i(z^3 + 6z^2 - 15z + 8)]$, in the neighbourhood of one of its saddle points; darker shading corresponds to larger magnitudes. The plot also shows the two level lines (thick solid lines) through the saddle and part of the line of steepest descents (dashed line) passing over it. At the saddle point, the angle between the line of steepest descents and a level line is $\pi/4$.

level lines of the function. It follows that the direction in which the magnitude of $h(z)$ changes most rapidly at any point z is in a direction perpendicular to the level line passing through that point. This is therefore the line through z on which the phase of $h(z)$, namely $\psi(z)$, is constant. Lines of constant phase are therefore sometimes referred to as *lines of steepest descent* (or steepest ascent).

We further note that $|h(z)|$ can never be negative and that neither ϕ nor ψ can have a finite maximum at any point at which $f(z)$ is analytic. This latter observation follows from the fact that at a maximum of, say, $\phi(x, y)$, both $\partial^2\phi/\partial x^2$ and $\partial^2\phi/\partial y^2$ would have to be negative; if this were so, Laplace's equation could not be satisfied, leading to a contradiction. A similar argument shows that a minimum of either ϕ or ψ is not possible wherever $f(z)$ is analytic. A more positive conclusion is that, since the two unmixed second partial derivatives $\partial^2\phi/\partial x^2$ and $\partial^2\phi/\partial y^2$ must have opposite signs, the only possible conclusion about a point at which $\nabla\phi$ is defined and equal to zero is that the point is a saddle point of $h(z)$. An example of a saddle point is shown as a greyscale plot in figure 25.12 and, more pictorially, in figure 5.2.

From the observations contained in the two previous paragraphs, we deduce that a path that follows the lines of steepest descent (or ascent) can never form a closed loop. On such a path, ϕ, and hence $|h(z)|$, must continue to decrease (increase) until the path meets a singularity of $f(z)$. It also follows that if a level line of $h(z)$ forms a closed loop in the complex plane, then the loop must enclose a singularity of $f(z)$. This may (if $\phi \to \infty$) or may not (if $\phi \to -\infty$) produce a singularity in $h(z)$.

We now turn to the study of the behaviour of $h(z)$ at a saddle point and how this enables us to find an approximation to the integral of $h(z)$ along a contour that can be deformed to pass through the saddle point. At a saddle point z_0, at which $f'(z_0) = 0$, both $\nabla\phi$ and $\nabla\psi$ are zero, and consequently the magnitude and phase of $h(z)$ are both stationary. The Taylor expansion of $f(z)$ at such a point takes the form

$$f(z) = f(z_0) + 0 + \frac{1}{2!} f''(z_0)(z - z_0)^2 + \mathrm{O}(z - z_0)^3. \tag{25.60}$$

We assume that $f''(z_0) \neq 0$ and write it explicitly as $f''(z_0) \equiv Ae^{i\alpha}$, thus defining the real quantities A and α. If it happens that $f''(z_0) = 0$, then two or more saddle points coalesce and the Taylor expansion must be continued until the first non-vanishing term is reached; we will not consider this case further, though the general method of proceeding will be apparent from what follows. If we also abbreviate the (in general) complex quantity $f(z_0)$ to f_0, then (25.60) takes the form

$$f(z) = f_0 + \tfrac{1}{2}Ae^{i\alpha}(z - z_0)^2 + \mathrm{O}(z - z_0)^3. \tag{25.61}$$

To study the implications of this approximation for $h(z)$, we write $z - z_0$ as $\rho\, e^{i\theta}$ with ρ and θ both real. Then

$$|h(z)| = |\exp(f_0)|\, \exp[\tfrac{1}{2}A\rho^2 \cos(2\theta + \alpha) + \mathrm{O}(\rho^3)]. \tag{25.62}$$

This shows that there are four values of θ for which $|h(z)|$ is independent of ρ (to second order). These therefore correspond to two crossing level lines given by

$$\theta = \tfrac{1}{2}\left(\pm\tfrac{1}{2}\pi - \alpha\right) \text{ and } \theta = \tfrac{1}{2}\left(\pm\tfrac{3}{2}\pi - \alpha\right). \tag{25.63}$$

The two level lines cross at right angles to each other. It should be noted that the continuations of the two level lines away from the saddle are not straight in general. At the saddle they have to satisfy (25.63), but away from it the lines must take whatever directions are needed to make $\nabla\phi = 0$. In figure 25.12 one of the level lines ($|h| = 1$) has a continuation ($y = 0$) that is straight; the other does not and bends away from its initial direction $x = 1$.

So far as the phase of $h(z)$ is concerned, we have

$$\arg[h(z)] = \arg(f_0) + \tfrac{1}{2}A\rho^2 \sin(2\theta + \alpha) + \mathrm{O}(\rho^3),$$

which shows that there are four other directions (two lines crossing at right

angles) in which the phase of $h(z)$ is independent of ρ. They make angles of $\pi/4$ with the level lines through z_0 and are given by

$$\theta = -\tfrac{1}{2}\alpha, \quad \theta = \tfrac{1}{2}(\pm\pi - \alpha), \quad \theta = \pi - \tfrac{1}{2}\alpha.$$

From our previous discussion it follows that these four directions will be the lines of steepest descent (or ascent) on moving away from the saddle point. In particular, the two directions for which the term $\cos(2\theta + \alpha)$ in (25.62) is *negative* will be the directions in which $|h(z)|$ *decreases* most rapidly from its value at the saddle point. These two directions are antiparallel, and a steepest descents path following them is a smooth locally straight line passing the saddle point. It is known as the *line of steepest descents* (l.s.d.) through the saddle point. Note that 'descents' is plural as on this line the value of $|h(z)|$ decreases on *both* sides of the saddle. This is the line which we will make the path of the contour integral of $h(z)$ follow. Part of a typical l.s.d. is indicated by the dashed line in figure 25.12.

25.8.2 Steepest descents method

To help understand how an integral along the line of steepest descents can be handled in a mechanical way, it is instructive to consider the case where the function $f(z) = -\beta z^2$ and $h(z) = \exp(-\beta z^2)$. The saddle point is situated at $z = z_0 = 0$, with $f_0 = f(z_0) = 1$ and $f''(z_0) = -2\beta$, implying that $A = 2|\beta|$ and $\alpha = \pm\pi + \arg\beta$, with the $\pm$ sign chosen to put α in the range $0 \leq \alpha < 2\pi$. Then the l.s.d. is determined by the requirement that $\sin(2\theta+\alpha) = 0$ whilst $\cos(2\theta+\alpha)$ is negative; together these imply that, for the l.s.d., $\theta = -\frac{1}{2}\arg\beta$ or $\theta = \pi - \frac{1}{2}\arg\beta$.

Since the Taylor series for $f(z) = -\beta z^2$ terminates after three terms, expansion (25.61) for this particular function is not an approximation to $h(z)$, but is exact. Consequently, a contour integral starting and endingin regions of the complex plane where the function tends to zero and following the l.s.d. through the saddle point at $z = 0$ will not only have a straight-line path, but will yield an exact result. Setting $z = te^{-\frac{1}{2}\arg\beta}$ will reduce the integral to that of a Gaussian function:

$$e^{-\frac{1}{2}\arg\beta}\int_{-\infty}^{\infty} e^{-|\beta|t^2}\,dt = e^{-\frac{1}{2}\arg\beta}\sqrt{\frac{\pi}{|\beta|}}.$$

The saddle-point method for a more general function aims to simulate this approach by deforming the integration contour C and forcing it to pass through a saddle point $z = z_0$, where, whatever the function, the leading z-dependent term in the exponent will be a quadratic function of $z - z_0$, thus turning the integrand into one that can be approximated by a Gaussian.

The path well away from the saddle point may be changed in any convenient way so long as it remains within the relevant sectors, as determined by the end-points of C. By a 'sector' we mean a region of the complex plane, any part of which can be reached from any other part of the same region without crossing

any of the continuations to infinity of the level lines that pass through the saddle. In practical applications the start- and end-points of the path are nearly always at singularities of $f(z)$ with $\mathrm{Re}\, f(z) \to -\infty$ and $|h(z)| \to 0$.

We now set out the complete procedure for the simplest form of integral evaluation that uses a method of steepest descents. Extensions, such as including higher terms in the Taylor expansion or having to pass through more than one saddle point in order to have appropriate termination points for the contour, can be incorporated, but the resulting calculations tend to be long and complicated, and we do not have space to pursue them in a book such as this one.

As our general integrand we take a function of the form $g(z)h(z)$, where, as before, $h(z) = \exp[f(z)]$. The function $g(z)$ should neither vary rapidly nor have zeros or singularities close to any saddle point used to evaluate the integral. Rapidly varying factors should be incorporated in the exponent, usually in the form of a logarithm. Provided $g(z)$ satisfies these criteria, it is sufficient to treat it as a constant multiplier when integrating, assigning to it its value at the saddle point, $g(z_0)$.

Incorporating this and retaining only the first two non-vanishing terms in equation (25.61) gives the integrand as

$$g(z_0)\exp(f_0)\exp[\tfrac{1}{2}Ae^{i\alpha}(z-z_0)^2]. \tag{25.64}$$

From the way in which it was defined, it follows that on the l.s.d. the imaginary part of $f(z)$ is constant (= Im f_0) and that the final exponent in (25.64) is either zero (at z_0) or negative. We can therefore write it as $-s^2$, where s is real. Further, since $\exp[f(z)] \to 0$ at the start- and end-points of the contour, we must have that s runs from $-\infty$ to $+\infty$, the sense of s being chosen so that it is negative approaching the saddle and positive when leaving it.

Making this change of variable,

$$\tfrac{1}{2}Ae^{i\alpha}(z-z_0)^2 = -s^2, \text{ with } dz = \pm\sqrt{\frac{2}{A}}\exp[\tfrac{1}{2}i(\pi-\alpha)]\,ds, \tag{25.65}$$

allows us to express the contribution to the integral from the neighbourhood of the saddle point as

$$\pm g(z_0)\exp(f_0)\sqrt{\frac{2}{A}}\exp[\tfrac{1}{2}i(\pi-\alpha)]\int_{-\infty}^{\infty}\exp(-s^2)\,ds.$$

The simple saddle-point approximation assumes that this is the only contribution, and gives as the value of the contour integral

$$\int_C g(z)\exp[f(z)]\,dz = \pm\sqrt{\frac{2\pi}{A}}\,g(z_0)\exp(f_0)\exp[\tfrac{1}{2}i(\pi-\alpha)], \tag{25.66}$$

where we have used the standard result that $\int_{-\infty}^{\infty}\exp(-s^2)\,ds = \sqrt{\pi}$. The overall $\pm$

sign is determined by the direction θ in the complex plane in which the distorted contour passes through the saddle point. If $-\frac{1}{2}\pi < \theta \leq \frac{1}{2}\pi$, then the positive sign is taken; if not, then the negative sign is appropriate. In broad terms, if the integration path through the saddle is in the direction of an increasing real part for z, then the overall sign is positive.

Formula (25.66) is the main result from a steepest descents approach to evaluating a contour integral of the type considered, in the sense that it is the leading term in any more refined calculation of the same integral. As can be seen, it is as an 'omnibus' formula, the various components of which can be found by considering a number of separate, less-complicated, calculations.

Before presenting a worked example that generates a substantial result, useful in another connection, it is instructive to consider an integral that can be simply and exactly evaluated by other means and then apply the saddle-point result to it. Of course, the steepest descents method will appear heavy-handed, but our purpose is to show it in action and to try to see why it works.

Consider the real integral

$$I = \int_{-\infty}^{\infty} \exp(10t - t^2)\, dt.$$

This can be evaluated directly by making the substitution $s = t - 5$ as follows:

$$I = \int_{-\infty}^{\infty} \exp(10t - t^2)\, dt = \int_{-\infty}^{\infty} \exp(25 - s^2)\, ds = e^{25} \int_{-\infty}^{\infty} \exp(-s^2)\, ds = \sqrt{\pi} e^{25}.$$

The saddle-point approach to the same problem is to consider the integral as a contour integral in the complex plane, but one that lies along the real axis. The saddle points of the integrand occur where $f'(t) = 10 - 2t = 0$; there is thus a single saddle point at $t = t_0 = 5$. This is on the real axis, and no distortion of the contour is necessary. The value f_0 of the exponent is $f(5) = 50 - 25 = 25$, whilst its second derivative at the saddle point is $f''(5) = -2$. Thus, $A = 2$ and $\alpha = \pi$. The contour clearly passes through the saddle point in the direction $\theta = 0$, i.e. in the positive sense on the real axis, and so the overall sign must be $+$. Since $g(t_0)$ is formally unity, we have all the ingredients needed for substitution in formula (25.66), which reads

$$I = +\sqrt{\frac{2\pi}{2}}\, 1 \exp(25) \exp[\tfrac{1}{2} i(\pi - \pi)] = \sqrt{\pi} e^{25}.$$

As it happens, this is exactly the same result as that obtained by accurate calculation. This would not normally be the case, but here it is, because of the quadratic nature of $10t - t^2$; all of its derivatives beyond the second are identically zero and no approximation of the exponent is involved.

Given the very large value of the integrand at the saddle point itself, the reader may wonder whether there really is a saddle there. However, evaluating the integrand at points lying on a line through the saddle point perpendicular

to the l.s.d., i.e. on the imaginary t-axis, provides some reassurance. Whether μ is positive or negative,

$$h(5+i\mu) = \exp(50 + 10i\mu - 25 - 10i\mu + \mu^2) = \exp(25+\mu^2).$$

This is greater than $h(5)$ for all μ and increases as $|\mu|$ increases, showing that the integration path really does lie at a minimum of $h(t)$ for a traversal in this direction.

We now give a fully worked solution to a problem that could not be easily tackled by elementary means.

► *Apply the saddle-point method to the function defined by*

$$F(x) = \frac{1}{\pi}\int_0^\infty \cos(\tfrac{1}{3}s^3 + xs)\,ds$$

to show that its form for large positive real x is one that tends asymptotically to zero, hence enabling $F(x)$ to be identified with the Airy function, $\mathrm{Ai}(x)$.

We first express the integral as an exponential function and then make the change of variable $s = x^{1/2}t$ to bring it into the canonical form $\int g(t)\exp[f(t)]\,dt$ as follows:

$$\begin{aligned} F(x) &= \frac{1}{\pi}\int_0^\infty \cos(\tfrac{1}{3}s^3 + xs)\,ds \\ &= \frac{1}{2\pi}\int_{-\infty}^\infty \exp[\,i(\tfrac{1}{3}s^3 + xs)\,]\,ds \\ &= \frac{1}{2\pi}\int_{-\infty}^\infty x^{1/2}\exp[\,ix^{3/2}(\tfrac{1}{3}t^3 + t)\,]\,dt. \end{aligned}$$

We now seek to find an approximate expression for this contour integral by deforming its path along the real t-axis into one passing over a saddle point of the integrand. Considered as a function of t, the multiplying factor $x^{1/2}/2\pi$ is a constant, and any effects due to the proximity of its zeros and singularities to any saddle point do not arise.

The saddle points are situated where

$$0 = f'(t) = ix^{3/2}(t^2+1) \quad \Rightarrow \quad t = \pm i.$$

For reasons discussed later, we choose to use the saddle point at $t = t_0 = i$. At this point,

$$f(i) = ix^{3/2}(-\tfrac{1}{3}i + i) = -\tfrac{2}{3}x^{3/2} \text{ and } Ae^{i\alpha} \equiv f''(i) = ix^{3/2}(2i) = -2x^{3/2},$$

and so $A = 2x^{3/2}$ and $\alpha = \pi$.

Now, expanding $f(t)$ around $t = i$ by setting $t = i + \rho\, e^{i\theta}$, we have

$$\begin{aligned} f(t) &= f(i) + 0 + \frac{1}{2!}f''(i)(t-i)^2 + \mathrm{O}[\,(t-i)^3\,] \\ &= -\frac{2}{3}x^{3/2} + \frac{1}{2}\,2x^{3/2}e^{i\pi}\rho^2 e^{2i\theta} + \mathrm{O}(\rho^3). \end{aligned}$$

For the l.s.d. contour that crosses the saddle point we need the second term in this last line to decrease as ρ increases. This happens if $\pi + 2\theta = \pm\pi$, i.e. if $\theta = 0$ or $\theta = -\pi$ (or $+\pi$); thus, the l.s.d. through the saddle is orientated parallel to the real t-axis. Given the initial contour direction, the deformed contour should approach the saddle point from the direction $\theta = -\pi$ and leave it along the line $\theta = 0$. Since $-\pi/2 < 0 \le \pi/2$, the overall sign of the 'omnibus' approximation formula is determined as positive.

Finally, putting the various values into the formula yields

$$\begin{aligned} F(x) &\sim + \left(\frac{2\pi}{A}\right)^{1/2} g(i) \exp[f(i)] \exp[\tfrac{1}{2}i(\pi - \alpha)] \\ &= + \left(\frac{2\pi}{2x^{3/2}}\right)^{1/2} \frac{x^{1/2}}{2\pi} \exp\left(-\frac{2}{3}x^{3/2}\right) \exp[\tfrac{1}{2}i(\pi - \pi)] \\ &= \frac{1}{2\sqrt{\pi}x^{1/4}} \exp\left(-\frac{2}{3}x^{3/2}\right). \end{aligned}$$

This is the leading term in the asymptotic expansion of $F(x)$, which, as shown in equation (25.39), is a particular contour integral solution of Stokes' equation. The fact that it tends to zero in a monotonic way as $x \to +\infty$ allows it to be identified with the Airy function, $\mathrm{Ai}(x)$.

We may ask why the saddle point at $t = -i$ was not used. The answer to this is as follows. Of course, any path that starts and ends in the right sectors will suffice, but if another saddle point exists close to the one used, then the Taylor expansion actually employed is likely to be less effective than if there were no other saddle points or if there were only distant ones.

An investigation of the same form as that used at $t = +i$ shows that the saddle at $t = -i$ is higher by a factor of $\exp(\frac{4}{3}x^{3/2})$ and that its l.s.d. is orientated parallel to the imaginary t-axis. Thus a path that went through it would need to go via a region of largish negative imaginary t, over the saddle at $t = -i$, and then, when it reached the col at $t = +i$, bend sharply and follow part of the same l.s.d. as considered earlier. Thus the contribution from the $t = -i$ saddle would be incomplete and roughly half of that from the $t = +i$ saddle would still have to be included. The more serious error would come from the first of these, as, clearly, the part of the path that lies in the plane $\mathrm{Re}\, t = 0$ is not symmetric and is far from Guassian-like on the side nearer the origin. The Gaussian-path approximation used will therefore not be a good one, and, what is more, the resulting error will be magnified by a factor $\exp(\frac{4}{3}x^{3/2})$ compared with the best estimate. So, both on the grounds of simplicity and because the effect of the other (neglected) saddle point is likely to be less severe, we choose to use the one at $t = +i$. ◀

25.8.3 Stationary phase method

In the previous subsection we showed how to use the saddle points of an exponential function of a complex variable to evaluate approximately a contour integral of that function. This was done by following the lines of steepest descent that passed through the saddle point; these are lines on which the phase of the exponential is constant but its amplitude is varying at the maximum possible rate for that function. We now introduce an alternative method, one that entirely reverses the roles of amplitude and phase. To see how such an alternative approach might work, it is useful to study how the integral of an exponential function of a complex variablecan be represented as the sum of infinitesimal vectors in the complex plane.

We start by studying the familiar integral

$$I_0 = \int_{-\infty}^{\infty} \exp(-z^2)\, dz, \tag{25.67}$$

which we already know has the value $\sqrt{\pi}$ when z is real. This choice of demonstration model is not accidental, but is motivated by the fact that, as we have already shown, in the neighbourhood of a saddle point all exponential integrands can be approximated by a Gaussian function of this form.

The same integral can also be thought of as an integral in the complex plane, in which the integration contour happens to be along the real axis. Since the integrand is analytic, the contour could be distorted into any other that had the same end-points, $z = -\infty$ and $z = +\infty$, both on the real axis.

As a particular possibility, we consider an arc of a circle of radius R centred on $z = 0$. It is easily shown that $\cos 2\theta \geq 1 + 4\theta/\pi$ for $-\pi/4 < \theta \leq 0$, where θ is measured from the positive real z-axis and $-\pi < \theta \leq \pi$. It follows from writing $z = R\,e^{i\theta}$ on the arc that, if the arc is confined to the region $-\pi/4 < \theta \leq 0$ (actually, $|\theta| < \pi/4$ is sufficient), then the integral of $\exp(-z^2)$ tends to zero as $R \to \infty$ anywhere on the arc. A similar result holds for an arc confined to the region $||\theta| - \pi| < \pi/4$. We also note for future use that, for $\pi/4 < \theta < 3\pi/4$ or $-\pi/4 > \theta > -3\pi/4$, the integrand $\exp(-z^2)$ grows without limit as $R \to \infty$, and that the larger R is, the more precipitous is the 'drop or rise' in its value on crossing the four radial lines $\theta = \pm\pi/4$ and $\theta = \pm 3\pi/4$.

Now consider a contour that consists of an arc at infinity running from $\theta = \pi$ to $\theta = \pi - \alpha$ joined to a straight line, $\theta = -\alpha$, which passes through $z = 0$ and continues to infinity, where it in turn joins an arc at infinity running from $\theta = -\alpha$ to $\theta = 0$. This contour has the same start- and end-points as that used in I_0, and so the integral of $\exp(-z^2)$ along it must also have the value $\sqrt{\pi}$. As the contributions to the integral from the arcs vanish, provided $\alpha < \pi/4$, it follows that the integral of $\exp(-z^2)$ along the infinite line $\theta = -\alpha$ is $\sqrt{\pi}$. If we now take α arbitrarily close to $\pi/4$, we may substitute $z = s\exp(-i\pi/4)$ into (25.67) and obtain

$$\begin{aligned}\sqrt{\pi} &= \int_{-\infty}^{\infty} \exp(-z^2)\,dz \\ &= \exp(-i\pi/4) \int_{-\infty}^{\infty} \exp(is^2)\,ds \qquad (25.68) \\ &= \sqrt{2\pi}\exp(-i\pi/4)\left[\int_0^{\infty} \cos(\tfrac{1}{2}\pi u^2)\,du + i\int_0^{\infty} \sin(\tfrac{1}{2}\pi u^2)\,du\right]. \qquad (25.69)\end{aligned}$$

The final line was obtained by making a scale change $s = \sqrt{\pi/2}\,u$. This enables the two integrals to be identified with the Fresnel integrals $C(x)$ and $S(x)$,

$$C(x) = \int_0^x \cos(\tfrac{1}{2}\pi u^2)\,du \text{ and } S(x) = \int_0^x \sin(\tfrac{1}{2}\pi u^2)\,du,$$

mentioned on page 645. Equation (25.69) can be rewritten as

$$\frac{(1+i)\sqrt{\pi}}{\sqrt{2}} = \sqrt{2\pi}\,[\,C(\infty) + iS(\infty)\,],$$

from which it follows that $C(\infty) = S(\infty) = \frac{1}{2}$. Clearly, $C(-\infty) = S(-\infty) = -\frac{1}{2}$.

We are now in a position to examine these two equivalent ways of evaluating I_0 in terms of sums of infinitesmal vectors in the complex plane. When the integral $\int_{-\infty}^{\infty} \exp(-z^2)\,dz$ is evaluated as a real integral, or a complex one along the real z-axis, each element dz generates a vector of length $\exp(-z^2)\,dz$ in an Argand diagram, usually called the *amplitude–phase diagram* for the integral. For this integration, whilst all vector contributions lie along the real axis, they do differ in magnitude, starting vanishingly small, growing to a maximum length of $1 \times dz$, and then reducing until they are again vanishingly small. At any stage, their vector sum (in this case, the same as their algebraic sum) is a measure of the indefinite integral

$$I(x) = \int_{-\infty}^{x} \exp(-z^2)\,dz. \tag{25.70}$$

The total length of the vector sum when $x \to \infty$ is, of course, $\sqrt{\pi}$, and it should not be overlooked that the sum is a vector parallel to (actually coinciding with) the real axis in the amplitude–phase diagram. Formally this indicates that the integral is real. This 'ordinary' view of evaluating the integral generates the same amplitude–phase diagram as does the method of steepest descents. This is because for this particular integrand the l.s.d. never leaves the real axis.

Now consider the same integral evaluated using the form of equation (25.69). Here, each contribution, as the integration variable goes from u to $u + du$, is of the form

$$g(u)\,du = \cos(\tfrac{1}{2}\pi u^2)\,du + i\sin(\tfrac{1}{2}\pi u^2)\,du.$$

As infinitesimal vectors in the amplitude–phase diagram, *all* $g(u)\,du$ have the *same* magnitude du, but their directions change continuously. Near $u = 0$, where u^2 is small, the change is slow and each vector element is approximately equal to $\sqrt{2\pi}\exp(-i\pi/4)\,du$; these contributions are all in phase and add up to a significant vector contribution in the direction $\theta = -\pi/4$. This is illustrated by the central part of the curve in part (b) of figure 25.13, in which the amplitude–phase diagram for the 'ordinary' integration, discussed above, is drawn as part (a).

Part (b) of the figure also shows that the vector representing the indefinite integral (25.70) initially (s large and negative) spirals out, in a clockwise sense, from around the point $0 + i0$ in the amplitude–phase diagram and ultimately (s large and positive) spirals in, in an anticlockwise direction, to the point $\sqrt{\pi} + i0$. The total curve is called a Cornu spiral. In physical applications, such as the diffraction of light at a straight edge, the relevant limits of integration are typically $-\infty$ and some finite value x. Then, as can be seen, the resulting vector sum is complex in general, with its magnitude (the distance from $0 + i0$ to the point on the spiral corresponding to $z = x$) growing steadily for $x < 0$ but showing oscillations when $x > 0$.

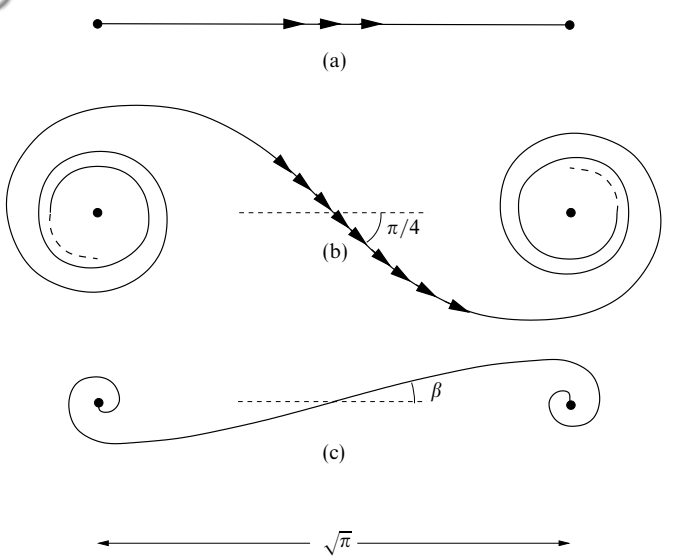


Figure 25.13 Amplitude–phase diagrams for the integral $\int_{-\infty}^{\infty} \exp(-z^2)\,dz$ using different contours in the complex z-plane. (a) Using the real axis, as in the steepest descents method. (b) Using the level line $z = u\exp(-\frac{1}{4}i\pi)$ that passes through the saddle point, as in the stationary phase method. (c) Using a path that makes a positive angle β ($< \pi/4$) with the z-axis.

The final curve, 25.13(c), shows the amplitude-phase diagram corresponding to an integration path that is along a line making a positive angle β ($0 < \beta < \pi/4$) with the real z-axis. In this case, the constituent infinitesimal vectors vary in both length and direction. Note that the curve passes through its centre point with the positive gradient $\tan\beta$ and that the directions of the spirals around the winding points are reversed as compared with case (b).

It is important to recognise that, although the three paths illustrated (and the infinity of other similar paths not illustrated) each produce a different phase–amplitude diagram, the vectors joining the initial and final points in the diagrams are *all the same*. For this particular integrand they are all (i) parallel to the positive real axis, showing that the integral is real and giving its sign, and (ii) of length $\sqrt{\pi}$, giving its magnitude.

What is apparent from figure 25.13(b), is that, because of the rapidly varying phase at either end of the spiral, the contributions from the infinitesimal vectors in those regions largely cancel each other. It is only in the central part of the spiral where the individual contributions are all nearly in phase that a substantial net contribution arises. If, on this part of the contour, where the phase is virtually

stationary, the magnitude of any factor, $g(z)$, multiplying the exponential function, $\exp[f(z)] \sim \exp[Ae^{i\alpha}(z-z_0)^2]$, is at least comparable to its magnitude elsewhere, then this result can be used to obtain an approximation to the value of the integral of $h(z) = g(z)\exp[f(z)]$. This is the basis of the method of stationary phase.

Returning to the behaviour of a function $\exp[f(z)]$ at one of its saddle points, we can now see how the considerations of the previous paragraphs can be applied there. We already know, from equation (25.62) and the discussion immediately following it, that in the equation

$$h(z) \approx g(z_0)\exp(f_0)\,\exp\{\tfrac{1}{2}A\rho^2[\cos(2\theta+\alpha)+i\sin(2\theta+\alpha)]\} \tag{25.71}$$

the second exponent is purely imaginary on a level line, and equal to zero at the saddle point itself. What is more, since $\nabla\psi = 0$ at the saddle, the phase is stationary there; on one level line it is a maximum and on the other it is a minimum. As there are two level lines through a saddle point, a path on which the amplitude of the integrand is constant could go straight on at the saddle point or it could turn through a right angle. For the moment we assume that it runs continuously through the saddle.

On the level line for which the phase at the saddle point is a minimum, we can write the phase of $h(z)$ as approximately

$$\arg g(z_0) + \operatorname{Im} f_0 + v^2,$$

where v is real, $iv^2 = \frac{1}{2}Ae^{i\alpha}(z-z_0)^2$ and, as previously, $Ae^{i\alpha} = f''(z_0)$. Then

$$e^{i\pi/4}\,dv = \pm\sqrt{\frac{A}{2}}\,e^{i\alpha/2}\,dz, \tag{25.72}$$

leading to an approximation to the integral of

$$\begin{aligned}\int h(z)\,dz &\approx \pm g(z_0)\exp(f_0)\int_{-\infty}^{\infty}\exp(iv^2)\sqrt{\frac{A}{2}}\,\exp[\,i(\tfrac{1}{4}\pi-\tfrac{1}{2}\alpha)\,]\,dv\\ &= \pm g(z_0)\exp(f_0)\sqrt{\pi}\,\exp(i\pi/4)\sqrt{\frac{A}{2}}\,\exp[\,i(\tfrac{1}{4}\pi-\tfrac{1}{2}\alpha)\,]\\ &= \pm\sqrt{\frac{2\pi}{A}}\,g(z_0)\exp(f_0)\exp[\,\tfrac{1}{2}i(\pi-\alpha)\,].\end{aligned} \tag{25.73}$$

Result (25.68) was used to obtain the second line above. The $\pm$ ambiguity is again resolved by the direction θ of the contour; it is positive if $-3\pi/4 < \theta \le \pi/4$; otherwise, it is negative.

What we have ignored in obtaining result (25.73) is that we have integrated along a level line and that therefore the integrand has the same magnitude far from the saddle as it has at the saddle itself. This could be dismissed by referring to the fact that contributions to the integral from the ends of the Cornu spiral

are self-cancelling, as discussed previously. However, the ends of the contour *must* be in regions where the integrand is vanishingly small, and so at each end of the level line we need to add a further section of path that makes the contour terminate correctly.

Fortunately, this can be done without adding to the value of the integral. This is because, as noted in the second paragraph following equation (25.67), far from the saddle the level line will be at a finite height up a 'precipitous cliff' that separates the region where the integrand grows without limit from the one where it tends to zero. To move down the cliff-face into the zero-level valley requires an ever smaller step the further we move away from the saddle; as the integrand is finite, the contribution to the integral is vanishingly small. In figure 25.12, this additional piece of path length might, for example, correspond to the infinitesimal move from a point on the large positive x-axis (where $h(z)$ has value 1) to a point just above it (where $h(z) \approx 0$).

Now that formula (25.73) has been justified, we may note that it is exactly the same as that for the method of steepest descents, equation (25.66). A similar calculation using the level line on which the phase is a maximum also reproduces the steepest-descents formula. It would appear that 'all roads lead to Rome'. However, as we explain later, some roads are more difficult than others. Where a problem involves using more than one saddle point, if the steepest-descents approach is tractable, it will usually be the more straight forward to apply.

Typical amplitude-phase diagrams for an integration along a level line that goes straight through the saddle are shown in parts (a) and (b) of figure 25.14. The value of the integral is given, in both magnitude and phase, by the vector $\mathbf{v}$ joining the initial to the final winding points and, of course, is the same in both cases. Part (a) corresponds to the case of the phase being a minimum at the saddle; the vector path crosses $\mathbf{v}$ at an angle of $-\pi/4$. When a path on which the phase at the saddle is a maximum is used, the Cornu spiral is as in part (b) of the figure; then the vector path crosses $\mathbf{v}$ at an angle of $+\pi/4$. As can be seen, the two spirals are mirror images of each other.

Clearly a straight-through level line path will start and end in different zero-level valleys. For one that turns through a right angle at the saddle point, the end-point could be in a different valley (for a function such as $\exp(-z^2)$, there is only one other) or in the same one. In the latter case the integral will give a zero value, unless a singularity of $h(z)$ happens to have been enclosed by the contour. Parts (c) and (d) of figure 25.14 illustrate the phase–amplitude diagrams for these two cases. In (c) the path turns through a right angle ($+\pi/2$, as it happens) at the saddle point, but finishes up in a different valley from that in which it started. In (d) it also turns through a right angle but returns to the same valley, albeit close to the other precipice from that near its starting point. This makes no difference and the result is zero, the two half spirals in the diagram producing resultants that cancel.

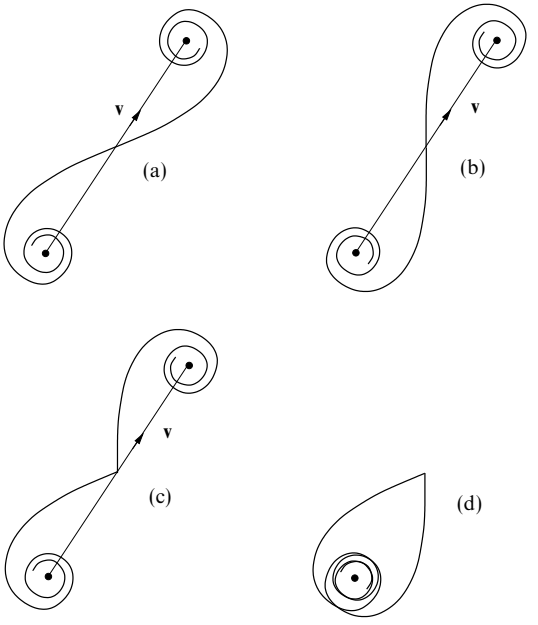


Figure 25.14 Amplitude–phase diagrams for stationary phase integration. (a) Using a straight-through path on which the phase is a minimum. (b) Using a straight-through path on which the phase is a maximum. (c) Using a level line that turns through $+\pi/2$ at the saddle point but starts and finishes in different valleys. (d) Using a level line that turns through a right angle but finishes in the same valley as it started. In cases (a), (b) and (c) the integral value is represented by $\mathbf{v}$ (see text). In case (d) the integral has value zero.

We do not have the space to consider cases with two or more saddle points, but even more care is needed with the stationary phase approach than when using the steepest-descents method. At a saddle point there is only one l.s.d. but there are two level lines. If more than one saddle point is required to reach the appropriate end-point of an integration, or an intermediate zero-level valley has to be used, then care is needed in linking the corresponding level lines in such a way that the links do not make a significant, but unknown, contribution to the integral. Yet more complications can arise if a level line through one saddle point crosses a line of steepest ascent through a second saddle.

We conclude this section with a worked example that has direct links to the two preceding sections of this chapter.

►*In the worked example in subsection 25.8.2 the function*

$$F(x) = \frac{1}{\pi}\int_0^\infty \cos(\tfrac{1}{3}s^3 + xs)\,ds \qquad (*)$$

was shown to have the properties associated with the Airy function, $\mathrm{Ai}(x)$*, when* $x > 0$*. Use the stationary phase method to show that, for* $x < 0$ *and* $-x$ *sufficiently large,*

$$F(x) \sim \frac{1}{\sqrt{\pi}(-x)^{1/4}}\,\sin\left[\frac{2}{3}(-x)^{3/2} + \frac{\pi}{4}\right],$$

in accordance with equation (25.53) for $\mathrm{Ai}(z)$*.*

Since the cosine function is an even function and its argument in (*) is purely real, we may consider $F(x)$ as the real part of

$$G(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp[\,i(\tfrac{1}{3}s^3 + xs)\,].$$

This is of the standard form for a saddle-point approach with $g(s) = 1/2\pi$ and $f(s) = i(\frac{1}{3}s^3 + xs)$. The latter has $f'(s) = 0$ when $s^2 = -x$. Since $x < 0$ there are two saddle points at $s = +\sqrt{-x}$ and $s = -\sqrt{-x}$. These are both on the real axis separated by a distance $2\sqrt{-x}$.

If $-x$ is sufficiently large, the Gaussian-like stationary phase integrals can be treated separately and their contributions simply added. In terms of a phase–amplitude diagram, the Cornu spiral from the first saddle will have effectively reached its final winding point before the spiral from the second saddle begins. The second spiral therefore takes the final point of the first as its starting point; the vector representing its net contribution need not be in the same direction as that arising from the first spiral, and in general it will not be.

Near the saddle at $s = +\sqrt{-x}$ the form of $f(s)$ is, in the usual notation,

$$\begin{aligned} f(s) &= f_0 + \tfrac{1}{2}Ae^{i\alpha}(s - s_0)^2 \\ &= -\frac{2i}{3}(-x)^{3/2} + \frac{1}{2}\,2\sqrt{-x}\,e^{i\pi/2}\,(\rho\,e^{i\theta})^2 \\ &= -\frac{2i}{3}(-x)^{3/2} + \sqrt{-x}\,e^{i\pi/2}\,\rho^2(\cos 2\theta + i\sin 2\theta). \end{aligned}$$

For the exponent to be purely imaginary requires $\sin 2\theta = 0$, implying that the level lines are given by $\theta = 0, \pi/2, \pi$ or $3\pi/2$. The same conclusions hold at the saddle at $s = -\sqrt{-x}$, which differs only in that the sign of f_0 is reversed and $\alpha = 3\pi/2$ rather than $\pi/2$; $\exp(i\alpha)$ is imaginary in both cases. Thus the obvious path is one that approaches both saddles from the direction $\theta = \pi$ and leaves them in the direction $\theta = 0$. As $-3\pi/4 < 0 < \pi/4$, the $\pm$ choice is resolved as positive at both saddles.

Next we calculate the approximate values of the integrals from equation (25.73). At $s = +\sqrt{-x}$ it is

$$\begin{aligned} &+\sqrt{\frac{2\pi}{2\sqrt{-x}}}\,\frac{1}{2\pi}\,\exp\left[-\frac{2i}{3}(-x)^{3/2}\right]\exp\left[\frac{i}{2}\left(\pi - \frac{\pi}{2}\right)\right] \\ &\quad = +\frac{1}{2\sqrt{\pi}(-x)^{1/4}}\,\exp\left[-i\left(\frac{2}{3}(-x)^{3/2} - \frac{\pi}{4}\right)\right]. \end{aligned}$$

The corresponding contribution from the saddle at $s = -\sqrt{-x}$ is

$$+\sqrt{\frac{2\pi}{2\sqrt{-x}}}\,\frac{1}{2\pi}\,\exp\left[\frac{2i}{3}(-x)^{3/2}\right]\exp\left[\frac{i}{2}\left(\pi - \frac{3\pi}{2}\right)\right],$$

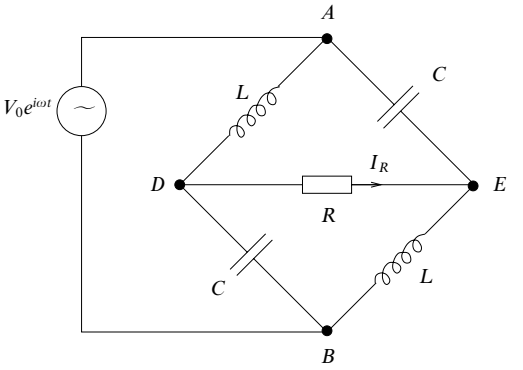


Figure 25.15 The inductor–capacitor–resistor network for exercise 25.1.

which can also be simplified, and gives

$$+\frac{1}{2\sqrt{\pi}(-x)^{1/4}}\exp\left[i\left(\frac{2}{3}(-x)^{3/2}-\frac{\pi}{4}\right)\right].$$

Adding the two contributions and taking the real part of the sum, though this is not necessary here because the sum is real anyway, we obtain

$$F(x)=\frac{2}{2\sqrt{\pi}(-x)^{1/4}}\cos\left(\frac{2}{3}(-x)^{3/2}-\frac{\pi}{4}\right)$$

$$=\frac{1}{\sqrt{\pi}(-x)^{1/4}}\sin\left(\frac{2}{3}(-x)^{3/2}+\frac{\pi}{4}\right),$$

in agreement with the asymptotic form given in (25.53). ◄

25.9 Exercises

25.1 In the method of complex impedances for a.c. circuits, an inductance L is represented by a complex impedance $Z_L = i\omega L$ and a capacitance C by $Z_C = 1/(i\omega C)$. Kirchhoff's circuit laws,

$$\sum_i I_i = 0 \text{ at a node and } \sum_i Z_i I_i = \sum_j V_j \text{ around any closed loop,}$$

are then applied as if the circuit were a d.c. one.

Apply this method to the a.c. bridge connected as in figure 25.15 to show that if the resistance R is chosen as $R = (L/C)^{1/2}$ then the amplitude of the current, I_R, through it is independent of the angular frequency ω of the applied a.c. voltage $V_0\,e^{i\omega t}$.

Determine how the phase of I_R, relative to that of the voltage source, varies with the angular frequency ω.

25.2 A long straight fence made of conducting wire mesh separates two fields and stands one metre high. Sometimes, on fine days, there is a vertical electric field over flat open countryside. Well away from the fence the strength of the field is E_0. By considering the effect of the transformation $w = (1-z^2)^{1/2}$ on the real and

imaginary z-axes, find the strengths of the field (a) at a point one metre directly above the fence, (b) at ground level one metre to the side of the fence, and (c) at a point that is level with the top of the fence but one metre to the side of it. What is the direction of the field in case (c)?

25.3 For the function

$$f(z) = \ln\left(\frac{z+c}{z-c}\right),$$

where c is real, show that the real part u of f is constant on a circle of radius $c\,\mathrm{cosech}\,u$ centred on the point $z = c\coth u$. Use this result to show that the electrical capacitance per unit length of two parallel cylinders of radii a, placed with their axes $2d$ apart, is proportional to $[\cosh^{-1}(d/a)]^{-1}$.

25.4 Find a complex potential in the z-plane appropriate to a physical situation in which the half-plane $x > 0$, $y = 0$ has zero potential and the half-plane $x < 0$, $y = 0$ has potential V.

By making the transformation $w = a(z + z^{-1})/2$, with a real and positive, find the electrostatic potential associated with the half-plane $r > a$, $s = 0$ and the half-plane $r < -a$, $s = 0$ at potentials 0 and V, respectively.

25.5 By considering in turn the transformations

$$z = \tfrac{1}{2}c(w + w^{-1}) \quad \text{and} \quad w = \exp\zeta,$$

where $z = x + iy$, $w = r\exp i\theta$, $\zeta = \xi + i\eta$ and c is a real positive constant, show that $z = c\cosh\zeta$ maps the strip $\xi \geq 0$, $0 \leq \eta \leq 2\pi$, onto the whole z-plane. Which curves in the z-plane correspond to the lines $\xi =$ constant and $\eta =$ constant? Identify those corresponding to $\xi = 0$, $\eta = 0$ and $\eta = 2\pi$.

The electric potential ϕ of a charged conducting strip $-c \leq x \leq c$, $y = 0$, satisfies

$$\phi \sim -k\ln(x^2 + y^2)^{1/2} \text{ for large values of } (x^2 + y^2)^{1/2},$$

with ϕ constant on the strip. Show that $\phi = \mathrm{Re}[-k\cosh^{-1}(z/c)]$ and that the magnitude of the electric field near the strip is $k(c^2 - x^2)^{-1/2}$.

25.6 For the equation $8z^3 + z + 1 = 0$:

(a) show that all three roots lie between the circles $|z| = 3/8$ and $|z| = 5/8$;
(b) find the approximate location of the real root, and hence deduce that the complex ones lie in the first and fourth quadrants and have moduli greater than 0.5.

25.7 Use contour integration to answer the following questions about the complex zeros of a polynomial equation.

(a) Prove that $z^8 + 3z^3 + 7z + 5$ has two zeros in the first quadrant.
(b) Find in which quadrants the zeros of $2z^3 + 7z^2 + 10z + 6$ lie. Try to locate them.

25.8 The following is a method of determining the number of zeros of an nth-degree polynomial $f(z)$ inside the contour C given by $|z| = R$:

(a) put $z = R(1 + it)/(1 - it)$, with $t = \tan(\theta/2)$, in the range $-\infty \leq t \leq \infty$;
(b) obtain $f(z)$ as

$$\frac{A(t) + iB(t)}{(1 - it)^n}\frac{(1 + it)^n}{(1 + it)^n};$$

(c) it follows that $\arg f(z) = \tan^{-1}(B/A) + n\tan^{-1}t$;
(d) and that $\Delta_C[\arg f(z)] = \Delta_C[\tan^{-1}(B/A)] + n\pi$;
(e) determine $\Delta_C[\tan^{-1}(B/A)]$ by evaluating $\tan^{-1}(B/A)$ at $t = \pm\infty$ and finding the discontinuities in B/A by inspection or using a sketch graph.

Then, by the principle of the argument, the number of zeros inside C is given by the integer $(2\pi)^{-1}\Delta_C[\arg f(z)]$.

It can be shown that the zeros of $z^4 + z + 1$ lie one in each quadrant. Use the above method to show that the zeros in the second and third quadrants have $|z| < 1$.

25.9 Prove that

$$\sum_{-\infty}^{\infty} \frac{1}{n^2 + \frac{3}{4}n + \frac{1}{8}} = 4\pi.$$

Carry out the summation numerically, say between -4 and 4, and note how much of the sum comes from values near the poles of the contour integration.

25.10 This exercise illustrates a method of summing some infinite series.

(a) Determine the residues at all the poles of the function

$$f(z) = \frac{\pi \cot \pi z}{a^2 + z^2},$$

where a is a positive real constant.

(b) By evaluating, in two different ways, the integral I of $f(z)$ along the straight line joining $-\infty - ia/2$ and $+\infty - ia/2$, show that

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

(c) Deduce the value of $\sum_1^{\infty} n^{-2}$.

25.11 By considering the integral of

$$\left(\frac{\sin \alpha z}{\alpha z}\right)^2 \frac{\pi}{\sin \pi z}, \qquad \alpha < \frac{\pi}{2},$$

around a circle of large radius, prove that

$$\sum_{m=1}^{\infty} (-1)^{m-1} \frac{\sin^2 m\alpha}{(m\alpha)^2} = \frac{1}{2}.$$

25.12 Use the Bromwich inversion, and contours similar to that shown in figure 25.7(a), to find the functions of which the following are the Laplace transforms:

(a) $s(s^2 + b^2)^{-1}$;
(b) $n!(s - a)^{-(n+1)}$, with n a positive integer and $s > a$;
(c) $a(s^2 - a^2)^{-1}$, with $s > |a|$.

Compare your answers with those given in a table of standard Laplace transforms.

25.13 Find the function $f(t)$ whose Laplace transform is

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

25.14 A function $f(t)$ has the Laplace transform

$$F(s) = \frac{1}{2i} \ln\left(\frac{s + i}{s - i}\right),$$

the complex logarithm being defined by a finite branch cut running along the imaginary axis from $-i$ to i.

(a) Convince yourself that, for $t > 0$, $f(t)$ can be expressed as a closed contour integral that encloses only the branch cut.

(b) Calculate $F(s)$ on either side of the branch cut, evaluate the integral and hence determine $f(t)$.
(c) Confirm that the derivative with respect to s of the Laplace transform integral of your answer is the same as that given by dF/ds.

25.15 Use the contour in figure 25.7(c) to show that the function with Laplace transform $s^{-1/2}$ is $(\pi x)^{-1/2}$.

[For an integrand of the form $r^{-1/2}\exp(-rx)$ change variable to $t = r^{1/2}$.]

25.16 Transverse vibrations of angular frequency ω on a string stretched with constant tension T are described by $u(x,t) = y(x)\,e^{-i\omega t}$, where

$$\frac{d^2y}{dx^2} + \frac{\omega^2 m(x)}{T}\,y(x) = 0.$$

Here, $m(x) = m_0 f(x)$ is the mass per unit length of the string and, in the general case, is a function of x. Find the first-order W.K.B. solution for $y(x)$.

Due to imperfections in its manufacturing process, a particular string has a small periodic variation in its linear density of the form $m(x) = m_0[1 + \epsilon\sin(2\pi x/L)]$, where $\epsilon \ll 1$. A progressive wave (i.e. one in which no energy is lost) travels in the positive x-direction along the string. Show that its amplitude fluctuates by $\pm\frac{1}{4}\epsilon$ of its value A_0 at $x = 0$ and that, to first order in ϵ, the phase of the wave is

$$\frac{\epsilon\,\omega\,L}{2\pi}\sqrt{\frac{m_0}{T}}\,\sin^2\frac{\pi x}{L}$$

ahead of what it would be if the string were uniform, with $m(x) = m_0$.

25.17 The equation

$$\frac{d^2y}{dz^2} + \left(\nu + \frac{1}{2} - \frac{1}{4}z^2\right)y = 0,$$

sometimes called the Weber–Hermite equation, has solutions known as parabolic cylinder functions. Find, to within (possibly complex) multiplicative constants, the two W.K.B. solutions of this equation that are valid for large $|z|$. In each case, determine the leading term and show that the multiplicative correction factor is of the form $1 + \mathrm{O}(\nu^2/z^2)$.

Identify the Stokes and anti-Stokes lines for the equation. On which of the Stokes lines is the W.K.B. solution that tends to zero for z large, real and negative, the dominant solution?

25.18 A W.K.B. solution of Bessel's equation of order zero,

$$\frac{d^2y}{dz^2} + \frac{1}{z}\frac{dy}{dz} + y = 0, \qquad (*)$$

valid for large $|z|$ and $-\pi/2 < \arg z < 3\pi/2$, is $y(z) = Az^{-1/2}e^{iz}$. Obtain an improvement on this by finding a multiplier of $y(z)$ in the form of an asymptotic expansion in inverse powers of z as follows.

(a) Substitute for $y(z)$ in (*) and show that the equation is satisfied to $\mathrm{O}(z^{-5/2})$.
(b) Now replace the constant A by $A(z)$ and find the equation that must be satisfied by $A(z)$. Look for a solution of the form $A(z) = z^{\sigma}\sum_{n=0}^{\infty} a_n z^{-n}$, where $a_0 = 1$. Show that $\sigma = 0$ is the only acceptable solution to the indicial equation and obtain a recurrence relation for the a_n.
(c) To within a (complex) constant, the expression $y(z) = A(z)z^{-1/2}e^{iz}$ is the asymptotic expansion of the Hankel function $H_0^{(1)}(z)$. Show that it is a divergent expansion for all values of z and estimate, in terms of z, the value of N such that $\sum_{n=0}^{N} a_n z^{-n-1/2}e^{iz}$ gives the best estimate of $H_0^{(1)}(z)$.

25.19 The function $h(z)$ of the complex variable z is defined by the integral

$$h(z) = \int_{-i\infty}^{i\infty} \exp(t^2 - 2zt)\, dt.$$

(a) Make a change of integration variable, $t = iu$, and evaluate $h(z)$ using a standard integral. Is your answer valid for all finite z?

(b) Evaluate the integral using the method of steepest descents, considering in particular the cases (i) z is real and positive, (ii) z is real and negative and (iii) z is purely imaginary and equal to $i\beta$, where β is real. In each case sketch the corresponding contour in the complex t-plane.

(c) Evaluate the integral for the same three cases as specified in part (b) using the method of stationary phases. To determine an appropriate contour that passes through a saddle point $t = t_0$, write $t = t_0 + (u + iv)$ and apply the criterion for determining a level line. Sketch the relevant contour in each case, indicating what freedom there is to distort it.

Comment on the accuracy of the results obtained using the approximate methods adopted in (b) and (c).

25.20 Use the method of steepest descents to show that an approximate value for the integral

$$F(z) = \int_{-\infty}^{\infty} \exp[\, iz(\tfrac{1}{5}t^5 + t)\,]\, dt,$$

where z is real and positive, is

$$\left(\frac{2\pi}{z}\right)^{1/2} \exp(-\beta z)\, \cos(\beta z - \tfrac{1}{8}\pi),$$

where $\beta = 4/(5\sqrt{2})$.

25.21 The stationary phase approximation to an integral of the form

$$F(v) = \int_a^b g(t) e^{ivf(t)}\, dt, \qquad |v| \gg 1,$$

where $f(t)$ is a real function of t and $g(t)$ is a slowly varying function (when compared with the argument of the exponential), can be written as

$$F(v) \sim \left(\frac{2\pi}{|v|}\right)^{1/2} \sum_{n=1}^{N} \frac{g(t_n)}{\sqrt{A_n}} \exp\left\{ i\left[\, vf(t_n) + \frac{\pi}{4}\, \mathrm{sgn}\Big(vf''(t_n)\Big)\,\right]\right\},$$

where the t_n are the N stationary points of $f(t)$ that lie in $a < t_1 < t_2 < \cdots < t_N < b$, $A_n = |\, f''(t_n)\,|$, and $\mathrm{sgn}(x)$ is the sign of x.

Use this result to find an approximation, valid for large positive values of v, to the integral

$$F(v, z) = \int_{-\infty}^{\infty} \frac{1}{1 + t^2}\, \cos[\,(2t^3 - 3zt^2 - 12z^2t)v\,]\, dt,$$

where z is a real positive parameter.

25.22 The Bessel function $J_v(z)$ is given for $|\arg z| < \frac{1}{2}\pi$ by the integral around a contour C of the function

$$g(z) = \frac{1}{2\pi i}\, t^{-(v+1)} \exp\left[\, \frac{z}{2}\left(t - \frac{1}{t}\right)\right].$$

The contour starts and ends along the negative real t-axis and encircles the origin in the positive sense. It can be considered to be made up of two contours. One of them, C_2, starts at $t = -\infty$, runs through the third quadrant to the point

$t = -i$ and then approaches the origin in the fourth quadrant in a curve that is ultimately antiparallel to the positive real axis. The other contour, C_1, is the mirror image of this in the real axis; it is confined to the upper half-plane, passes through $t = i$ and is antiparallel to the real t-axis at both of its extremities. The contribution to $J_\nu(z)$ from the curve C_k is $\frac{1}{2}H_\nu^{(k)}$, the function $H_\nu^{(k)}$ being known as a Hankel function.

Using the method of steepest descents, establish the leading term in an asymptotic expansion for $H_\nu^{(1)}$ for z real, large and positive. Deduce, without detailed calculation, the corresponding result for $H_\nu^{(2)}$. Hence establish the asymptotic form of $J_\nu(z)$ for the same range of z.

25.23 Use the method of steepest descents to find an asymptotic approximation, valid for z large, real and positive, to the function defined by

$$F_\nu(z) = \int_C \exp(-iz\sin t + i\nu t)\,dt,$$

where ν is real and non-negative and C is a contour that starts at $t = -\pi + i\infty$ and ends at $t = -i\infty$.

25.10 Hints and answers

25.1 Apply Kirchhoff's laws to three independent loops, say $ADBA$, $ADEA$ and $DBED$. Eliminate other currents from the equations to obtain $I_R = \omega_0 C V_0[(\omega_0^2 - \omega^2 - 2i\omega\omega_0)/(\omega_0^2 + \omega^2)]$, where $\omega_0^2 = (LC)^{-1}$; $|I_R| = \omega_0 C V_0$; the phase of I_R is $\tan^{-1}[(-2\omega\omega_0)/(\omega_0^2 - \omega^2)]$.

25.3 Set $c\coth u_1 = -d$, $c\coth u_2 = +d$, $|c\,\mathrm{cosech}\,u| = a$ and note that the capacitance is proportional to $(u_2 - u_1)^{-1}$.

25.5 $\xi =$ constant, ellipses $x^2(a+1)^{-2} + y^2(a-1)^{-2} = c^2/(4a^2)$; $\eta =$ constant, hyperbolae $x^2(\cos\alpha)^{-2} - y^2(\sin\alpha)^{-2} = c^2$. The curves are the cuts $-c \le x \le c$, $y = 0$ and $|x| \ge c$, $y = 0$. The curves for $\eta = 2\pi$ are the same as those for $\eta = 0$.

25.7 (a) For a quarter-circular contour enclosing the first quadrant, the change in the argument of the function is $0 + 8(\pi/2) + 0$ (since $y^8 + 5 = 0$ has no real roots); (b) one negative real zero; a conjugate pair in the second and third quadrants, $-\frac{3}{2}$, $-1 \pm i$.

25.9 Evaluate

$$\int \frac{\pi\cot\pi z}{(\frac{1}{2}+z)(\frac{1}{4}+z)}\,dz$$

around a large circle centred on the origin; residue at $z = -1/2$ is 0; residue at $z = -1/4$ is $4\pi\cot(-\pi/4)$.

25.11 The behaviour of the integrand for large $|z|$ is $|z|^{-2}\exp[(2\alpha - \pi)|z|]$. The residue at $z = \pm m$, for each integer m, is $\sin^2(m\alpha)(-1)^m/(m\alpha)^2$. The contour contributes nothing.
Required summation $=$ [total sum $-$ ($m = 0$ term)]/2.

25.13 Note that $\bar{f}(s)$ has no pole at $s = 0$. For $t < 0$ close the Bromwich contour in the right half-plane, and for $t > 1$ in the left half-plane. For $0 < t < 1$ the integrand has to be split into separate terms containing e^{-s} and $s - 1$ and the completions made in the right and left half-planes, respectively. The last of these completed contours now contains a second-order pole at $s = 0$. $f(t) = 1 - t$ for $0 < t < 1$, but is 0 otherwise.

25.15 $\int_\Gamma$ and $\int_\gamma$ tend to 0 as $R \to \infty$ and $\rho \to 0$. Put $s = r\exp i\pi$ and $s = r\exp(-i\pi)$ on the two sides of the cut and use $\int_0^\infty \exp(-t^2x)\,dt = \frac{1}{2}(\pi/x)^{1/2}$. There are no poles inside the contour.

25.17 Use the binomial theorem to expand, in inverse powers of z, both the square root in the exponent and the fourth root in the multiplier, working to $O(z^{-2})$. The leading terms are $y_1(z) = Ce^{-z^2/4}z^{\nu}$ and $y_2(z) = De^{z^2/4}z^{-(\nu+1)}$. Stokes lines: $\arg z = 0, \pi/2, \pi, 3\pi/2$; anti-Stokes lines: $\arg z = (2n+1)\pi/4$ for $n = 0, 1, 2, 3$. y_1 is dominant on $\arg z = \pi/2$ or $3\pi/2$.

25.19 (a) $i\sqrt{\pi}e^{-z^2}$, valid for all z, including $i\sqrt{\pi}\exp(\beta^2)$ in case (iii).
(b) The same values as in (a). The (only) saddle point, at $t_0 = z$, is traversed in the direction $\theta = +\frac{1}{2}\pi$ in all cases, though the path in the complex t-plane varies with each case.
(c) The same values as in (a). The level lines are $v = \pm u$. In cases (i) and (ii) the contour turns through a right angle at the saddle point.
All three methods give *exact* answers in this case of a quadratic exponent.

25.21 Saddle points at $t_1 = -z$ and $t_2 = 2z$ with $f_1'' = -18z$ and $f_2'' = 18z$. Approximation is

$$\left(\frac{\pi}{9zv}\right)^{1/2}\left[\frac{\cos(7vz^3 - \frac{1}{4}\pi)}{1+z^2} + \frac{\cos(20vz^3 - \frac{1}{4}\pi)}{1+4z^2}\right].$$

25.23 Saddle point at $t_0 = \cos^{-1}(v/z)$ is traversed in the direction $\theta = -\frac{1}{4}\pi$. $F_v(z) \approx (2\pi/z)^{1/2}\exp[i(z - \frac{1}{2}v\pi - \frac{1}{4}\pi)]$.

26

Tensors

It may seem obvious that the quantitative description of physical processes cannot depend on the coordinate system in which they are represented. However, we may turn this argument around: since physical results must indeed be independent of the choice of coordinate system, what does this imply about the nature of the quantities involved in the description of physical processes? The study of these implications and of the classification of physical quantities by means of them forms the content of the present chapter.

Although the concepts presented here may be applied, with little modification, to more abstract spaces (most notably the four-dimensional space–time of special or general relativity), we shall restrict our attention to our familiar three-dimensional Euclidean space. This removes the need to discuss the properties of differentiable manifolds and their tangent and dual spaces. The reader who is interested in these more technical aspects of tensor calculus in general spaces, and in particular their application to general relativity, should consult one of the many excellent textbooks on the subject.[§]

Before the presentation of the main development of the subject, we begin by introducing the summation convention, which will prove very useful in writing tensor equations in a more compact form. We then review the effects of a change of basis in a vector space; such spaces were discussed in chapter 8. This is followed by an investigation of the rotation of Cartesian coordinate systems, and finally we broaden our discussion to include more general coordinate systems and transformations.

[§] For example, R. D'Inverno, *Introducing Einstein's Relativity* (Oxford: Oxford University Press, 1992); J. Foster and J. D. Nightingale, *A Short Course in General Relativity* (New York: Springer, 2006); B. F. Schutz, *A First Course in General Relativity* (Cambridge; Cambridge University Press 1985).

26.1 Some notation

Before proceeding further, we introduce the *summation convention* for subscripts, since its use looms large in the work of this chapter. The convention is that any *lower-case* alphabetic subscript that appears *exactly* twice in any term of an expression is understood to be summed over all the values that a subscript in that position can take (unless the contrary is specifically stated). The subscripted quantities may appear in the numerator and/or the denominator of a term in an expression. This naturally implies that any such pair of repeated subscripts must occur only in subscript positions that have the same range of values. Sometimes the ranges of values have to be specified but usually they are apparent from the context.

The following simple examples illustrate what is meant (in the three-dimensional case):

(i) $a_i x_i$ stands for $a_1x_1 + a_2x_2 + a_3x_3$;

(ii) $a_{ij}b_{jk}$ stands for $a_{i1}b_{1k} + a_{i2}b_{2k} + a_{i3}b_{3k}$;

(iii) $a_{ij}b_{jk}c_k$ stands for $\sum_{j=1}^{3}\sum_{k=1}^{3} a_{ij}b_{jk}c_k$;

(iv) $\dfrac{\partial v_i}{\partial x_i}$ stands for $\dfrac{\partial v_1}{\partial x_1} + \dfrac{\partial v_2}{\partial x_2} + \dfrac{\partial v_3}{\partial x_3}$;

(v) $\dfrac{\partial^2 \phi}{\partial x_i \partial x_i}$ stands for $\dfrac{\partial^2 \phi}{\partial x_1^2} + \dfrac{\partial^2 \phi}{\partial x_2^2} + \dfrac{\partial^2 \phi}{\partial x_3^2}$.

Subscripts that are summed over are called *dummy subscripts* and the others *free subscripts*. It is worth remarking that when introducing a dummy subscript into an expression, care should be taken not to use one that is already present, either as a free or as a dummy subscript. For example, $a_{ij}b_{jk}c_{kl}$ cannot, and must not, be replaced by $a_{ij}b_{jj}c_{jl}$ or by $a_{il}b_{lk}c_{kl}$, but could be replaced by $a_{im}b_{mk}c_{kl}$ or by $a_{im}b_{mn}c_{nl}$. Naturally, free subscripts must not be changed at all unless the working calls for it.

Furthermore, as we have done throughout this book, we will make frequent use of the Kronecker delta δ_{ij}, which is defined by

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

When the summation convention has been adopted, the main use of δ_{ij} is to replace one subscript by another in certain expressions. Examples might include

$$b_j\delta_{ij} = b_i,$$

and

$$a_{ij}\delta_{jk} = a_{ij}\delta_{kj} = a_{ik}. \tag{26.1}$$

In the second of these the dummy index shared by both terms on the left-hand side (namely j) has been replaced by the free index carried by the Kronecker delta (namely k), and the delta symbol has disappeared. In matrix language, (26.1) can be written as $\mathsf{AI} = \mathsf{A}$, where A is the matrix with elements a_{ij} and I is the unit matrix having the same dimensions as A.

In some expressions we may use the Kronecker delta to replace indices in a number of different ways, e.g.

$$a_{ij}b_{jk}\delta_{ki} = a_{ij}b_{ji} \quad \text{or} \quad a_{kj}b_{jk},$$

where the two expressions on the RHS are totally equivalent to one another.

26.2 Change of basis

In chapter 8 some attention was given to the subject of changing the basis set (or coordinate system) in a vector space and it was shown that, under such a change, different types of quantity behave in different ways. These results are given in section 8.15, but are summarised below for convenience, using the summation convention. Although throughout this section we will remind the reader that we are using this convention, it will simply be assumed in the remainder of the chapter.

If we introduce a set of basis vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ into our familiar three-dimensional (vector) space, then we can describe any vector $\mathbf{x}$ in terms of its components x_1, x_2, x_3 with respect to this basis:

$$\mathbf{x} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + x_3\mathbf{e}_3 = x_i\mathbf{e}_i,$$

where we have used the summation convention to write the sum in a more compact form. If we now introduce a new basis $\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3$ related to the old one by

$$\mathbf{e}'_j = S_{ij}\mathbf{e}_i \qquad \text{(sum over } i\text{)}, \tag{26.2}$$

where the coefficient S_{ij} is the ith component of the vector $\mathbf{e}'_j$ with respect to the unprimed basis, then we may write $\mathbf{x}$ with respect to the new basis as

$$\mathbf{x} = x'_1\mathbf{e}'_1 + x'_2\mathbf{e}'_2 + x'_3\mathbf{e}'_3 = x'_i\mathbf{e}'_i \qquad \text{(sum over } i\text{)}.$$

If we denote the matrix with elements S_{ij} by S, then the components x'_i and x_i in the two bases are related by

$$x'_i = (\mathsf{S}^{-1})_{ij}x_j \qquad \text{(sum over } j\text{)},$$

where, using the summation convention, there is an implicit sum over j from $j = 1$ to $j = 3$. In the special case where the transformation is a rotation of the coordinate axes, the transformation matrix S is orthogonal and we have

$$x'_i = (\mathsf{S}^{\mathrm{T}})_{ij}x_j = S_{ji}x_j \qquad \text{(sum over } j\text{)}. \tag{26.3}$$

Scalars behave differently under transformations, however, since they remain unchanged. For example, the value of the scalar product of two vectors $\mathbf{x} \cdot \mathbf{y}$ (which is just a number) is unaffected by the transformation from the unprimed to the primed basis. Different again is the behaviour of linear operators. If a linear operator $\mathcal{A}$ is represented by some matrix A in a given coordinate system then in the new (primed) coordinate system it is represented by a new matrix, $\mathsf{A}' = \mathsf{S}^{-1}\mathsf{A}\mathsf{S}$.

In this chapter we develop a general formulation to describe and classify these different types of behaviour under a change of basis (or coordinate transformation). In the development, the generic name *tensor* is introduced, and certain scalars, vectors and linear operators are described respectively as tensors of zeroth, first and second order (the *order* – or *rank* – corresponds to the number of subscripts needed to specify a particular element of the tensor). Tensors of third and fourth order will also occupy some of our attention.

26.3 Cartesian tensors

We begin our discussion of tensors by considering a particular class of coordinate transformation – namely rotations – and we shall confine our attention strictly to the rotation of Cartesian coordinate systems. Our object is to study the properties of various types of mathematical quantities, and their associated physical interpretations, when they are described in terms of Cartesian coordinates and the axes of the coordinate system are rigidly rotated from a basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ (lying along the Ox_1, Ox_2 and Ox_3 axes) to a new one $\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3$ (lying along the Ox'_1, Ox'_2 and Ox'_3 axes).

Since we shall be more interested in how the components of a vector or linear operator are changed by a rotation of the axes than in the relationship between the two sets of basis vectors $\mathbf{e}_i$ and $\mathbf{e}'_i$, let us define the transformation matrix L as the inverse of the matrix S in (26.2). Thus, from (26.2), the components of a position vector $\mathbf{x}$, in the old and new bases respectively, are related by

$$x'_i = L_{ij}x_j. \tag{26.4}$$

Because we are considering only rigid rotations of the coordinate axes, the transformation matrix L will be orthogonal, i.e. such that $\mathsf{L}^{-1} = \mathsf{L}^{\mathrm{T}}$. Therefore the inverse transformation is given by

$$x_i = L_{ji}x'_j. \tag{26.5}$$

The orthogonality of L also implies relations among the elements of L that express the fact that $\mathsf{L}\mathsf{L}^{\mathrm{T}} = \mathsf{L}^{\mathrm{T}}\mathsf{L} = \mathsf{I}$. In subscript notation they are given by

$$L_{ik}L_{jk} = \delta_{ij} \qquad \text{and} \qquad L_{ki}L_{kj} = \delta_{ij}. \tag{26.6}$$

Furthermore, in terms of the basis vectors of the primed and unprimed Cartesian

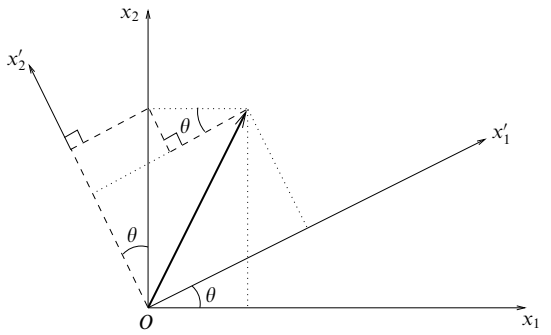


Figure 26.1 Rotation of Cartesian axes by an angle θ about the x_3-axis. The three angles marked θ and the parallels (broken lines) to the primed axes show how the first two equations of (26.7) are constructed.

coordinate systems, the transformation matrix is given by

$$L_{ij} = \mathbf{e}_i' \cdot \mathbf{e}_j.$$

We note that the product of two rotations is also a rotation. For example, suppose that $x_i' = L_{ij}x_j$ and $x_i'' = M_{ij}x_j'$; then the composite rotation is described by

$$x_i'' = M_{ij}x_j' = M_{ij}L_{jk}x_k = (\mathsf{ML})_{ik}x_k,$$

corresponding to the matrix ML.

►*Find the transformation matrix* L *corresponding to a rotation of the coordinate axes through an angle* θ *about the* $\mathbf{e}_3$*-axis (or* x_3*-axis), as shown in figure 26.1.*

Taking $\mathbf{x}$ as a position vector – the most obvious choice – we see from the figure that the components of $\mathbf{x}$ with respect to the new (primed) basis are given in terms of the components in the old (unprimed) basis by

$$\begin{aligned} x_1' &= x_1\cos\theta + x_2\sin\theta, \\ x_2' &= -x_1\sin\theta + x_2\cos\theta, \\ x_3' &= x_3. \end{aligned} \tag{26.7}$$

The (orthogonal) transformation matrix is thus

$$\mathsf{L} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The inverse equations are

$$\begin{aligned} x_1 &= x_1'\cos\theta - x_2'\sin\theta, \\ x_2 &= x_1'\sin\theta + x_2'\cos\theta, \\ x_3 &= x_3', \end{aligned} \tag{26.8}$$

in line with (26.5). ◄

26.4 First- and zero-order Cartesian tensors

Using the above example as a guide, we may consider any set of three quantities v_i, which are directly or indirectly functions of the coordinates x_i and possibly involve some constants, and ask how their values are changed by any rotation of the Cartesian axes. The specific question to be answered is whether the specific forms v_i' in the new variables can be obtained from the old ones v_i using (26.4),

$$v_i' = L_{ij}v_j. \tag{26.9}$$

If so, the v_i are said to form the components of a *vector* or *first-order Cartesian tensor* **v**. By definition, the position coordinates are themselves the components of such a tensor.The first-order tensor **v** does not change under rotation of the coordinate axes; nevertheless, since the basis set does change, from $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ to $\mathbf{e}_1'$, $\mathbf{e}_2'$, $\mathbf{v}_3'$, the components of **v** must also change. The changes must be such that

$$\mathbf{v} = v_i\mathbf{e}_i = v_i'\mathbf{e}_i' \tag{26.10}$$

is unchanged.

Since the transformation (26.9) is orthogonal, the components of any such first-order Cartesian tensor also obey a relation that is the inverse of (26.9),

$$v_i = L_{ji}v_j'. \tag{26.11}$$

We now consider explicit examples. In order to keep the equations to reasonable proportions, the examples will be restricted to the x_1x_2-plane, i.e. there are no components in the x_3-direction. Three-dimensional cases are no different in principle – but much longer to write out.

►*Which of the following pairs* (v_1, v_2) *form the components of a first-order Cartesian tensor in two dimensions?:*

(i) $(x_2, -x_1)$, (ii) (x_2, x_1), (iii) (x_1^2, x_2^2).

We shall consider the rotation discussed in the previous example, and to save space we denote $\cos\theta$ by c and $\sin\theta$ by s.

(i) Here $v_1 = x_2$ and $v_2 = -x_1$, referred to the old axes. In terms of the new coordinates they will be $v_1' = x_2'$ and $v_2' = -x_1'$, i.e.

$$\begin{aligned} v_1' &= x_2' &&= -sx_1 + cx_2 \\ v_2' &= -x_1' &&= -cx_1 - sx_2. \end{aligned} \tag{26.12}$$

Now if we start again and evaluate v_1' and v_2' as given by (26.9) we find that

$$\begin{aligned} v_1' &= L_{11}v_1 + L_{12}v_2 &&= cx_2 + s(-x_1) \\ v_2' &= L_{21}v_1 + L_{22}v_2 &&= -s(x_2) + c(-x_1). \end{aligned} \tag{26.13}$$

The expressions for v_1' and v_2' in (26.12) and (26.13) are the same whatever the values of θ (i.e. for *all* rotations) and thus by definition (26.9) the pair $(x_2, -x_1)$ *is* a first-order Cartesian tensor.

(ii) Here $v_1 = x_2$ and $v_2 = x_1$. Following the same procedure,

$$v_1' = x_2' = -sx_1 + cx_2$$
$$v_2' = x_1' = cx_1 + sx_2.$$

But, by (26.9), for a Cartesian tensor we must have

$$v_1' = cv_1 + sv_2 = cx_2 + sx_1$$

$$v_2' = (-s)v_1 + cv_2 = -sx_2 + cx_1.$$

These two sets of expressions do not agree and thus the pair (x_2, x_1) is not a first-order Cartesian tensor.

(iii) $v_1 = x_1^2$ and $v_2 = x_2^2$. As in (ii) above, considering the first component alone is sufficient to show that this pair is also not a first-order tensor. Evaluating v_1' directly gives

$$v_1' = x_1'^2 = c^2x_1^2 + 2csx_1x_2 + s^2x_2^2,$$

whilst (26.9) requires that

$$v_1' = cv_1 + sv_2 = cx_1^2 + sx_2^2,$$

which is quite different. ◄

There are many physical examples of first-order tensors (i.e. vectors) that will be familiar to the reader. As a straightforward one, we may take the set of Cartesian components of the momentum of a particle of mass m, $(m\dot{x}_1, m\dot{x}_2, m\dot{x}_3)$. This set transforms in all essentials as (x_1, x_2, x_3), since the other operations involved, multiplication by a number and differentiation with respect to time, are quite unaffected by any orthogonal transformation of the axes. Similarly, acceleration and force are represented by the components of first-order tensors.

Other more complicated vectors involving the position coordinates more than once, such as the angular momentum of a particle of mass m, namely $\mathbf{J} = \mathbf{x} \times \mathbf{p} = m(\mathbf{x} \times \dot{\mathbf{x}})$, are also first-order tensors. That this is so is less obvious in component form than for the earlier examples, but may be verified by writing out the components of $\mathbf{J}$ explicitly or by appealing to the quotient law to be discussed in section 26.7 and using the Cartesian tensor ϵ_{ijk} from section 26.8.

Having considered the effects of rotations on vector-like sets of quantities we may consider quantities that are unchanged by a rotation of axes. In our previous nomenclature these have been called *scalars* but we may also describe them as *tensors of zero order*. They contain only one element (formally, the number of subscripts needed to identify a particular element is zero); the most obvious non-trivial example associated with a rotation of axes is the square of the distance of a point from the origin, $r^2 = x_1^2 + x_2^2 + x_3^2$. In the new coordinate system it will have the form $r'^2 = x_1'^2 + x_2'^2 + x_3'^2$, which for any rotation has the same value as $x_1^2 + x_2^2 + x_3^2$.

In fact any scalar product of two first-order tensors (vectors) is a zero-order tensor (scalar), as might be expected since it can be written in a coordinate-free way as $\mathbf{u} \cdot \mathbf{v}$.

►*By considering the components of the vectors* $\mathbf{u}$ *and* $\mathbf{v}$ *with respect to two Cartesian coordinate systems (related by a rotation), show that the scalar product* $\mathbf{u} \cdot \mathbf{v}$ *is invariant under rotation.*

In the original (unprimed) system the scalar product is given in terms of components by $u_i v_i$ (summed over i), and in the rotated (primed) system by

$$u_i' v_i' = L_{ij} u_j L_{ik} v_k = L_{ij} L_{ik} u_j v_k = \delta_{jk} u_j v_k = u_j v_j,$$

where we have used the orthogonality relation (26.6). Since the resulting expression in the rotated system is the same as that in the original system, the scalar product is indeed invariant under rotations. ◄

The above result leads directly to the identification of many physically important quantities as zero-order tensors. Perhaps the most immediate of these is energy, either as potential energy or as an energy density (e.g. $\mathbf{F} \cdot d\mathbf{r}$, $e\mathbf{E} \cdot d\mathbf{r}$, $\mathbf{D} \cdot \mathbf{E}$, $\mathbf{B} \cdot \mathbf{H}$, $\boldsymbol{\mu} \cdot \mathbf{B}$), but others, such as the angle between two directed quantities, are important.

As mentioned in the first paragraph of this chapter, in most analyses of physical situations it is a scalar quantity (such as energy) that is to be determined. Such quantities are *invariant* under a rotation of axes and so it is possible to work with the most convenient set of axes and still have confidence in the results.

Complementing the way in which a zero-order tensor was obtained from two first-order tensors, so a first-order tensor can be obtained from a zero-order tensor (i.e. a scalar). We show this by taking a specific example, that of the electric field $\mathbf{E} = -\nabla\phi$; this is derived from a scalar, the electrostatic potential ϕ, and has components

$$E_i = -\frac{\partial \phi}{\partial x_i}. \tag{26.14}$$

Clearly, $\mathbf{E}$ *is* a first-order tensor, but we may prove this more formally by considering the behaviour of its components (26.14) under a rotation of the coordinate axes, since the components of the electric field E_i' are then given by

$$E_i' = \left(-\frac{\partial \phi}{\partial x_i}\right)' = -\frac{\partial \phi'}{\partial x_i'} = -\frac{\partial x_j}{\partial x_i'}\frac{\partial \phi}{\partial x_j} = L_{ij} E_j, \tag{26.15}$$

where (26.5) has been used to evaluate $\partial x_j / \partial x_i'$. Now (26.15) is in the form (26.9), thus confirming that the components of the electric field do behave as the components of a first-order tensor.

►*If v_i are the components of a first-order tensor, show that $\nabla \cdot \mathbf{v} = \partial v_i/\partial x_i$ is a zero-order tensor.*

In the rotated coordinate system $\nabla \cdot \mathbf{v}$ is given by

$$\left(\frac{\partial v_i}{\partial x_i}\right)' = \frac{\partial v_i'}{\partial x_i'} = \frac{\partial x_j}{\partial x_i'}\frac{\partial}{\partial x_j}(L_{ik}v_k) = L_{ij}L_{ik}\frac{\partial v_k}{\partial x_j},$$

since the elements L_{ij} are not functions of position. Using the orthogonality relation (26.6) we then find

$$\frac{\partial v_i'}{\partial x_i'} = L_{ij}L_{ik}\frac{\partial v_k}{\partial x_j} = \delta_{jk}\frac{\partial v_k}{\partial x_j} = \frac{\partial v_j}{\partial x_j}.$$

Hence $\partial v_i/\partial x_i$ is invariant under rotation of the axes and is thus a zero-order tensor; this was to be expected since it can be written in a coordinate-free way as $\nabla \cdot \mathbf{v}$. ◄

26.5 Second- and higher-order Cartesian tensors

Following on from scalars with no subscripts and vectors with one subscript, we turn to sets of quantities that require two subscripts to identify a particular element of the set. Let these quantities by denoted by T_{ij}.

Taking (26.9) as a guide we define a *second-order Cartesian tensor* as follows: the T_{ij} form the components of such a tensor if, under the same conditions as for (26.9),

$$T_{ij}' = L_{ik}L_{jl}T_{kl} \tag{26.16}$$

and

$$T_{ij} = L_{ki}L_{lj}T_{kl}'. \tag{26.17}$$

At the same time we may define a Cartesian tensor of general order as follows. The set of expressions $T_{ij\ldots k}$ form the components of a Cartesian tensor if, for all rotations of the axes of coordinates given by (26.4) and (26.5), subject to (26.6), the expressions using the new coordinates, $T'_{ij\ldots k}$ are given by

$$T'_{ij\ldots k} = L_{ip}L_{jq}\cdots L_{kr}T_{pq\ldots r} \tag{26.18}$$

and

$$T_{ij\ldots k} = L_{pi}L_{qj}\cdots L_{rk}T'_{pq\ldots r}. \tag{26.19}$$

It is apparent that in three dimensions, an Nth-order Cartesian tensor has 3^N components.

Since a second-order tensor has two subscripts, it is natural to display its components in matrix form. The notation $[T_{ij}]$ is used, as well as T, to denote the matrix having T_{ij} as the element in the ith row and jth column.§

We may think of a second-order tensor $\mathbf{T}$ as a geometrical entity in a similar way to that in which we viewed linear operators (which transform one vector into

§ We can also denote the column matrix containing the elements v_i of a vector by $[v_i]$.

another, without reference to any coordinate system) and consider the matrix containing its components as a representation of the tensor with respect to a particular coordinate system. Moreover, the matrix $\mathsf{T} = [T_{ij}]$, containing the components of a second-order tensor, behaves in the same way under orthogonal transformations $\mathsf{T}' = \mathsf{L}\mathsf{T}\mathsf{L}^{\mathrm{T}}$ as a linear operator.

However, not all linear operators are second-order tensors. More specifically, the two subscripts in a second-order tensor must refer to the same coordinate system. In particular, this means that any linear operator that transforms a vector into a vector in a different vector space cannot be a second-order tensor. Thus, although the elements L_{ij} of the transformation matrix are written with two subscripts, they cannot be the components of a tensor since the two subscripts each refer to a different coordinate system.

As examples of sets of quantities that are readily shown to be second-order tensors we consider the following.

(i) *The outer product of two vectors.* Let u_i and v_i, $i = 1, 2, 3$, be the components of two vectors $\mathbf{u}$ and $\mathbf{v}$, and consider the set of quantities T_{ij} defined by

$$T_{ij} = u_i v_j. \tag{26.20}$$

The set T_{ij} are called the components of the the *outer product* of $\mathbf{u}$ and $\mathbf{v}$. Under rotations the components T_{ij} become

$$T'_{ij} = u'_i v'_j = L_{ik} u_k L_{jl} v_l = L_{ik} L_{jl} u_k v_l = L_{ik} L_{jl} T_{kl}, \tag{26.21}$$

which shows that they do transform as the components of a second-order tensor. Use has been made in (26.21) of the fact that u_i and v_i are the components of first-order tensors.

The outer product of two vectors is often denoted, without reference to any coordinate system, as

$$\mathbf{T} = \mathbf{u} \otimes \mathbf{v}. \tag{26.22}$$

(This is not to be confused with the vector product of two vectors, which is itself a vector and is discussed in chapter 7.) The expression (26.22) gives the basis to which the components T_{ij} of the second-order tensor refer: since $\mathbf{u} = u_i \mathbf{e}_i$ and $\mathbf{v} = v_i \mathbf{e}_i$, we may write the tensor $\mathbf{T}$ as

$$\mathbf{T} = u_i \mathbf{e}_i \otimes v_j \mathbf{e}_j = u_i v_j \mathbf{e}_i \otimes \mathbf{e}_j = T_{ij} \mathbf{e}_i \otimes \mathbf{e}_j. \tag{26.23}$$

Moreover, as for the case of first-order tensors (see equation (26.10)) we note that the quantities T'_{ij} are the components of the *same* tensor $\mathbf{T}$, but referred to a different coordinate system, i.e.

$$\mathbf{T} = T_{ij} \mathbf{e}_i \otimes \mathbf{e}_j = T'_{ij} \mathbf{e}'_i \otimes \mathbf{e}'_j.$$

These concepts can be extended to higher-order tensors.

(ii) *The gradient of a vector*. Suppose v_i represents the components of a vector; let us consider the quantities generated by forming the derivatives of each v_i, $i = 1, 2, 3$, with respect to each x_j, $j = 1, 2, 3$, i.e.

$$T_{ij} = \frac{\partial v_i}{\partial x_j}.$$

These nine quantities form the components of a second-order tensor, as can be seen from the fact that

$$T'_{ij} = \frac{\partial v'_i}{\partial x'_j} = \frac{\partial (L_{ik} v_k)}{\partial x_l} \frac{\partial x_l}{\partial x'_j} = L_{ik} \frac{\partial v_k}{\partial x_l} L_{jl} = L_{ik} L_{jl} T_{kl}.$$

In coordinate-free language the tensor $\mathbf{T}$ may be written as $\mathbf{T} = \nabla \mathbf{v}$ and hence gives meaning to the concept of the gradient of a vector, a quantity that was not discussed in the chapter on vector calculus (chapter 10).

A test of whether any given set of quantities forms the components of a second-order tensor can always be made by direct substitution of the x'_i in terms of the x_i, followed by comparison with the right-hand side of (26.16). This procedure is extremely laborious, however, and it is almost always better to try to recognise the set as being expressible in one of the forms just considered, or to make alternative tests based on the quotient law of section 26.7 below.

►*Show that the T_{ij} given by*

$$\mathsf{T} = [T_{ij}] = \begin{pmatrix} x_2^2 & -x_1 x_2 \\ -x_1 x_2 & x_1^2 \end{pmatrix} \tag{26.24}$$

are the components of a second-order tensor.

Again we consider a rotation θ about the $\mathbf{e}_3$-axis. Carrying out the direct evaluation first we obtain, using (26.7),

$$\begin{aligned}
T'_{11} &= x'^2_2 = s^2 x_1^2 - 2sc x_1 x_2 + c^2 x_2^2, \\
T'_{12} &= -x'_1 x'_2 = sc x_1^2 + (s^2 - c^2) x_1 x_2 - sc x_2^2, \\
T'_{21} &= -x'_1 x'_2 = sc x_1^2 + (s^2 - c^2) x_1 x_2 - sc x_2^2, \\
T'_{22} &= x'^2_1 = c^2 x_1^2 + 2sc x_1 x_2 + s^2 x_2^2.
\end{aligned}$$

Now, evaluating the right-hand side of (26.16),

$$\begin{aligned}
T'_{11} &= cc x_2^2 + cs(-x_1 x_2) + sc(-x_1 x_2) + ss x_1^2, \\
T'_{12} &= c(-s) x_2^2 + cc(-x_1 x_2) + s(-s)(-x_1 x_2) + sc x_1^2, \\
T'_{21} &= (-s) c x_2^2 + (-s) s(-x_1 x_2) + cc(-x_1 x_2) + cs x_1^2, \\
T'_{22} &= (-s)(-s) x_2^2 + (-s) c(-x_1 x_2) + c(-s)(-x_1 x_2) + cc x_1^2.
\end{aligned}$$

After reorganisation, the corresponding expressions are seen to be the same, showing, as required, that the T_{ij} are the components of a second-order tensor.

The same result could be inferred much more easily, however, by noting that the T_{ij} are in fact the components of the outer product of the vector $(x_2, -x_1)$ with itself. That $(x_2, -x_1)$ is indeed a vector was established by (26.12) and (26.13). ◄

Physical examples involving second-order tensors will be discussed in the later sections of this chapter, but we might note here that, for example, magnetic susceptibility and electrical conductivity are described by second-order tensors.

26.6 The algebra of tensors

Because of the similarity of first- and second-order tensors to column vectors and matrices, it would be expected that similar types of algebraic operation can be carried out with them and so provide ways of constructing new tensors from old ones. In the remainder of this chapter, instead of referring to the T_{ij} (say) as the *components* of a second-order tensor $\mathbf{T}$, we may sometimes simply refer to T_{ij} as the tensor. It should always be remembered, however, that the T_{ij} are in fact just the components of $\mathbf{T}$ in a given coordinate system and that T'_{ij} refers to the components of the *same* tensor $\mathbf{T}$ in a different coordinate system.

The addition and subtraction of tensors follows an obvious definition; namely that if $V_{ij\ldots k}$ and $W_{ij\ldots k}$ are (the components of) tensors of the same order, then their sum and difference, $S_{ij\ldots k}$ and $D_{ij\ldots k}$ respectively, are given by

$$\begin{aligned} S_{ij\ldots k} &= V_{ij\ldots k} + W_{ij\ldots k}, \\ D_{ij\ldots k} &= V_{ij\ldots k} - W_{ij\ldots k}, \end{aligned}$$

for each set of values $i, j, \ldots, k$. That $S_{ij\ldots k}$ and $D_{ij\ldots k}$ are the components of tensors follows immediately from the linearity of a rotation of coordinates.

It is equally straightforward to show that if the $T_{ij\ldots k}$ are the components of a tensor, then so is the set of quantities formed by interchanging the order of (a pair of) indices, e.g. $T_{ji\ldots k}$.

If $T_{ji\ldots k}$ is found to be identical with $T_{ij\ldots k}$ then $T_{ij\ldots k}$ is said to be *symmetric* with respect to its first two subscripts (or simply 'symmetric', for second-order tensors). If, however, $T_{ji\ldots k} = -T_{ij\ldots k}$ for every element then it is an *antisymmetric* tensor. An arbitrary tensor is neither symmetric nor antisymmetric but can always be written as the sum of a symmetric tensor $S_{ij\ldots k}$ and an antisymmetric tensor $A_{ij\ldots k}$:

$$\begin{aligned} T_{ij\ldots k} &= \tfrac{1}{2}(T_{ij\ldots k} + T_{ji\ldots k}) + \tfrac{1}{2}(T_{ij\ldots k} - T_{ji\ldots k}) \\ &= S_{ij\ldots k} + A_{ij\ldots k}. \end{aligned}$$

Of course these properties are valid for any pair of subscripts.

In (26.20) in the previous section we had an example of a kind of 'multiplication' of two tensors, thereby producing a tensor of higher order – in that case two first-order tensors were multiplied to give a second-order tensor. Inspection of (26.21) shows that there is nothing particular about the orders of the tensors involved and it follows as a general result that the outer product of an Nth-order tensor with an Mth-order tensor will produce an $(M + N)$th-order tensor.

An operation that produces the opposite effect – namely, generates a tensor of smaller rather than larger order – is known as *contraction* and consists of making two of the subscripts equal and summing over all values of the equalised subscripts.

►*Show that the process of contraction of an Nth-order tensor produces another tensor, of order* $N-2$.

Let $T_{ij\ldots l\ldots m\ldots k}$ be the components of an Nth-order tensor, then

$$T'_{ij\ldots l\ldots m\ldots k} = \underbrace{L_{ip}L_{jq}\cdots L_{lr}\cdots L_{ms}\cdots L_{kn}}_{N \text{ factors}} T_{pq\ldots r\ldots s\ldots n}.$$

Thus if, for example, we make the two subscripts l and m equal and sum over all values of these subscripts, we obtain

$$\begin{aligned} T'_{ij\ldots l\ldots l\ldots k} &= L_{ip}L_{jq}\cdots L_{lr}\cdots L_{ls}\cdots L_{kn}T_{pq\ldots r\ldots s\ldots n} \\ &= L_{ip}L_{jq}\cdots \delta_{rs}\cdots L_{kn}T_{pq\ldots r\ldots s\ldots n} \\ &= \underbrace{L_{ip}L_{jq}\cdots L_{kn}}_{(N-2) \text{ factors}} T_{pq\ldots r\ldots r\ldots n}, \end{aligned}$$

showing that $T_{ij\ldots l\ldots l\ldots k}$ are the components of a (different) Cartesian tensor of order $N-2$. ◄

For a second-rank tensor, the process of contraction is the same as taking the trace of the corresponding matrix. The trace T_{ii} itself is thus a zero-order tensor (or scalar) and hence invariant under rotations, as was noted in chapter 8.

The process of taking the scalar product of two vectors can be recast into tensor language as forming the outer product $T_{ij} = u_i v_j$ of two first-order tensors $\mathbf{u}$ and $\mathbf{v}$ and then contracting the second-order tensor $\mathbf{T}$ so formed, to give $T_{ii} = u_i v_i$, a scalar (invariant under a rotation of axes).

As yet another example of a familiar operation that is a particular case of a contraction, we may note that the multiplication of a column vector $[u_i]$ by a matrix $[B_{ij}]$ to produce another column vector $[v_i]$,

$$B_{ij}u_j = v_i,$$

can be looked upon as the contraction T_{ijj} of the third-order tensor T_{ijk} formed from the outer product of B_{ij} and u_k.

26.7 The quotient law

The previous paragraph appears to give a heavy-handed way of describing a familiar operation, but it leads us to ask whether it has a converse. To put the question in more general terms: if we know that $\mathbf{B}$ and $\mathbf{C}$ are tensors and also that

$$A_{pq\cdots k\cdots m}B_{ij\cdots k\cdots n} = C_{pq\cdots mij\cdots n}, \tag{26.25}$$

does this imply that the $A_{pq\cdots k\cdots m}$ also form the components of a tensor **A**? Here **A**, **B** and **C** are respectively of Mth, Nth and $(M+N-2)$th order and it should be noted that the subscript k that has been contracted may be any of the subscripts in **A** and **B** independently.

The *quotient law* for tensors states that if (26.25) holds in all rotated coordinate frames then the $A_{pq\cdots k\cdots m}$ do indeed form the components of a tensor **A**. To prove it for general M and N is no more difficult regarding the ideas involved than to show it for specific M and N, but this does involve the introduction of a large number of subscript symbols. We will therefore take the case $M = N = 2$, but it will be readily apparent that the principle of the proof holds for general M and N.

We thus start with (say)

$$A_{pk}B_{ik} = C_{pi}, \tag{26.26}$$

where B_{ik} and C_{pi} are arbitrary second-order tensors. Under a rotation of coordinates the set A_{pk} (tensor or not) transforms into a new set of quantities that we will denote by A'_{pk}. We thus obtain in succession the following steps, using (26.16), (26.17) and (26.6):

$$\begin{aligned}
A'_{pk}B'_{ik} &= C'_{pi} && \text{(transforming (26.26)),}\\
&= L_{pq}L_{ij}C_{qj} && \text{(since } \mathbf{C} \text{ is a tensor),}\\
&= L_{pq}L_{ij}A_{ql}B_{jl} && \text{(from (26.26)),}\\
&= L_{pq}L_{ij}A_{ql}L_{mj}L_{nl}B'_{mn} && \text{(since } \mathbf{B} \text{ is a tensor),}\\
&= L_{pq}L_{nl}A_{ql}B'_{in} && \text{(since } L_{ij}L_{mj} = \delta_{im}\text{).}
\end{aligned}$$

Now k on the left and n on the right are dummy subscripts and thus we may write

$$(A'_{pk} - L_{pq}L_{kl}A_{ql})B'_{ik} = 0. \tag{26.27}$$

Since B_{ik}, and hence B'_{ik}, is an arbitrary tensor, we must have

$$A'_{pk} = L_{pq}L_{kl}A_{ql},$$

showing that the A'_{pk} are given by the general formula (26.18) and hence that the A_{pk} are the components of a second-order tensor. By following an analogous argument, the same result (26.27) and deduction could be obtained if (26.26) were replaced by

$$A_{pk}B_{ki} = C_{pi},$$

i.e. the contraction being now with respect to a different pair of indices.

Use of the quotient law to test whether a given set of quantities is a tensor is generally much more convenient than making a direct substitution. A particular way in which it is applied is by contracting the given set of quantities, having

N subscripts, with an arbitrary Nth-order tensor (i.e. one having independently variable components) and determining whether the result is a scalar.

► *Use the quotient law to show that the elements of* T*, equation (26.24), are the components of a second-order tensor.*

The outer product $x_i x_j$ is a second-order tensor. Contracting this with the T_{ij} given in (26.24) we obtain

$$T_{ij}x_i x_j = x_2^2 x_1^2 - x_1 x_2 x_1 x_2 - x_1 x_2 x_2 x_1 + x_1^2 x_2^2 = 0,$$

which is clearly invariant (a zeroth-order tensor). Hence by the quotient theorem T_{ij} must also be a tensor. ◄

26.8 The tensors δ_{ij} and ϵ_{ijk}

In many places throughout this book we have encountered and used the two-subscript quantity δ_{ij} defined by

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

Let us now also introduce the three-subscript *Levi–Civita symbol* ϵ_{ijk}, the value of which is given by

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } i,j,k \text{ is an even permutation of } 1,2,3, \\ -1 & \text{if } i,j,k \text{ is an odd permutation of } 1,2,3, \\ 0 & \text{otherwise.} \end{cases}$$

We will now show that δ_{ij} and ϵ_{ijk} are respectively the components of a second- and a third-order Cartesian tensor. Notice that the coordinates x_i do not appear explicitly in the components of these tensors, their components consisting entirely of 0 and 1.

In passing, we also note that ϵ_{ijk} is totally antisymmetric, i.e. it changes sign under the interchange of any pair of subscripts. In fact ϵ_{ijk}, or any scalar multiple of it, is the *only* three-subscript quantity with this property.

Treating δ_{ij} first, the proof that it is a second-order tensor is straightforward since if, from (26.16), we consider the equation

$$\delta'_{kl} = L_{ki}L_{lj}\delta_{ij} = L_{ki}L_{li} = \delta_{kl},$$

we see that the transformation of δ_{ij} generates the same expression (a pattern of 0's and 1's) as does the definition of δ'_{ij} in the transformed coordinates. Thus δ_{ij} transforms according to the appropriate tensor transformation law and is therefore a second-order tensor.

Turning now to ϵ_{ijk}, we have to consider the quantity

$$\epsilon'_{lmn} = L_{li}L_{mj}L_{nk}\epsilon_{ijk}. \tag{26.28}$$

Let us begin, however, by noting that we may use the Levi–Civita symbol to write an expression for the determinant of a 3×3 matrix A,

$$|\mathsf{A}|\epsilon_{lmn} = A_{li}A_{mj}A_{nk}\epsilon_{ijk}, \tag{26.29}$$

which may be shown to be equivalent to the Laplace expansion (see chapter 8).[§] Indeed many of the properties of determinants discussed in chapter 8 can be proved very efficiently using this expression (see exercise 26.9).

►*Evaluate the determinant of the matrix*

$$\mathsf{A} = \begin{pmatrix} 2 & 1 & -3 \\ 3 & 4 & 0 \\ 1 & -2 & 1 \end{pmatrix}.$$

Setting $l = 1$, $m = 2$ and $n = 3$ in (26.29) we find

$$\begin{aligned} |\mathsf{A}| &= \epsilon_{ijk}A_{1i}A_{2j}A_{3k} \\ &= (2)(4)(1) - (2)(0)(-2) - (1)(3)(1) + (-3)(3)(-2) \\ &\quad + (1)(0)(1) - (-3)(4)(1) = 35, \end{aligned}$$

which may be verified using the Laplace expansion method. ◄

We can now show that the ϵ_{ijk} are in fact the components of a third-order tensor. Using (26.29) with the general matrix A replaced by the specific transformation matrix L, we can rewrite the RHS of (26.28) in terms of $|\mathsf{L}|$

$$\epsilon'_{lmn} = L_{li}L_{mj}L_{nk}\epsilon_{ijk} = |\mathsf{L}|\epsilon_{lmn}.$$

Since L is orthogonal its determinant has the value unity, and so $\epsilon'_{lmn} = \epsilon_{lmn}$. Thus we see that ϵ'_{lmn} has exactly the properties of ϵ_{ijk} but with i, j, k replaced by l, m, n, i.e. it is the same as the expression ϵ_{ijk} written using the new coordinates. This shows that ϵ_{ijk} is a third-order Cartesian tensor.

In addition to providing a convenient notation for the determinant of a matrix, δ_{ij} and ϵ_{ijk} can be used to write many of the familiar expressions of vector algebra and calculus as contracted tensors. For example, provided we are using right-handed Cartesian coordinates, the vector product $\mathbf{a} = \mathbf{b} \times \mathbf{c}$ has as its ith component $a_i = \epsilon_{ijk}b_jc_k$; this should be contrasted with the outer product $\mathbf{T} = \mathbf{b} \otimes \mathbf{c}$, which is a second-order tensor having the components $T_{ij} = b_ic_j$.

[§] This may be readily extended to an $N \times N$ matrix A, i.e.

$$|\mathsf{A}|\epsilon_{i_1i_2\cdots i_N} = A_{i_1j_1}A_{i_2j_2}\cdots A_{i_Nj_N}\epsilon_{j_1j_2\cdots j_N},$$

where $\epsilon_{i_1i_2\cdots i_N}$ equals 1 if $i_1i_2\cdots i_N$ is an even permutation of $1, 2, \ldots, N$ and equals -1 if it is an odd permutation; otherwise it equals zero.

► *Write the following as contracted Cartesian tensors:* $\mathbf{a}\cdot\mathbf{b}$, $\nabla^2\phi$, $\nabla\times\mathbf{v}$, $\nabla(\nabla\cdot\mathbf{v})$, $\nabla\times(\nabla\times\mathbf{v})$, $(\mathbf{a}\times\mathbf{b})\cdot\mathbf{c}$.

The corresponding (contracted) tensor expressions are readily seen to be as follows:

$$\mathbf{a}\cdot\mathbf{b} = a_i b_i \;=\; \delta_{ij}a_i b_j,$$

$$\nabla^2\phi = \frac{\partial^2\phi}{\partial x_i \partial x_i} \;=\; \delta_{ij}\frac{\partial^2\phi}{\partial x_i \partial x_j},$$

$$(\nabla\times\mathbf{v})_i = \epsilon_{ijk}\frac{\partial v_k}{\partial x_j},$$

$$[\nabla(\nabla\cdot\mathbf{v})]_i = \frac{\partial}{\partial x_i}\left(\frac{\partial v_j}{\partial x_j}\right) \;=\; \delta_{jk}\frac{\partial^2 v_j}{\partial x_i \partial x_k},$$

$$[\nabla\times(\nabla\times\mathbf{v})]_i = \epsilon_{ijk}\frac{\partial}{\partial x_j}\left(\epsilon_{klm}\frac{\partial v_m}{\partial x_l}\right) \;=\; \epsilon_{ijk}\epsilon_{klm}\frac{\partial^2 v_m}{\partial x_j \partial x_l},$$

$$(\mathbf{a}\times\mathbf{b})\cdot\mathbf{c} = \delta_{ij}c_i\epsilon_{jkl}a_k b_l \;=\; \epsilon_{ikl}c_i a_k b_l. \;\blacktriangleleft$$

An important relationship between the ϵ- and δ- tensors is expressed by the identity

$$\epsilon_{ijk}\epsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}. \tag{26.30}$$

To establish the validity of this identity between two fourth-order tensors (the LHS is a once-contracted sixth-order tensor) we consider the various possible cases.

The RHS of (26.30) has the values

$$+1 \text{ if } i = l \text{ and } j = m \neq i, \tag{26.31}$$

$$-1 \text{ if } i = m \text{ and } j = l \neq i, \tag{26.32}$$

$$0 \text{ for any other set of subscript values } i, j, l, m. \tag{26.33}$$

In each product on the LHS k has the same value in both factors and for a non-zero contribution none of i, l, j, m can have the same value as k. Since there are only three values, 1, 2 and 3, that any of the subscripts may take, the only non-zero possibilities are $i = l$ and $j = m$ or vice versa but not all four subscripts equal (since then each ϵ factor is zero, as it would be if $i = j$ or $l = m$). This reproduces (26.33) for the LHS of (26.30) and also the conditions (26.31) and (26.32). The values in (26.31) and (26.32) are also reproduced in the LHS of (26.30) since

(i) if $i = l$ and $j = m$, $\epsilon_{ijk} = \epsilon_{lmk} = \epsilon_{klm}$ and, whether ϵ_{ijk} is $+1$ or -1, the product of the two factors is $+1$; and

(ii) if $i = m$ and $j = l$, $\epsilon_{ijk} = \epsilon_{mlk} = -\epsilon_{klm}$ and thus the product $\epsilon_{ijk}\epsilon_{klm}$ (no summation) has the value -1.

This concludes the establishment of identity (26.30).

A useful application of (26.30) is in obtaining alternative expressions for vector quantities that arise from the vector product of a vector product.

►*Obtain an alternative expression for* $\nabla \times (\nabla \times \mathbf{v})$.

As shown in the previous example, $\nabla \times (\nabla \times \mathbf{v})$ can be expressed in tensor form as

$$\begin{aligned}[\nabla \times (\nabla \times \mathbf{v})]_i &= \epsilon_{ijk}\epsilon_{klm}\frac{\partial^2 v_m}{\partial x_j \partial x_l} \\ &= (\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})\frac{\partial^2 v_m}{\partial x_j \partial x_l} \\ &= \frac{\partial}{\partial x_i}\left(\frac{\partial v_j}{\partial x_j}\right) - \frac{\partial^2 v_i}{\partial x_j \partial x_j} \\ &= [\nabla(\nabla \cdot \mathbf{v})]_i - \nabla^2 v_i,\end{aligned}$$

where in the second line we have used the identity (26.30). This result has already been mentioned in chapter 10 and the reader is referred there for a discussion of its applicability. ◄

By examining the various possibilities, it is straightforward to verify that, more generally,

$$\epsilon_{ijk}\epsilon_{pqr} = \begin{vmatrix} \delta_{ip} & \delta_{iq} & \delta_{ir} \\ \delta_{jp} & \delta_{jq} & \delta_{jr} \\ \delta_{kp} & \delta_{kq} & \delta_{kr} \end{vmatrix} \tag{26.34}$$

and it is easily seen that (26.30) is a special case of this result. From (26.34) we can derive alternative forms of (26.30), for example,

$$\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}. \tag{26.35}$$

The pattern of subscripts in these identities is most easily remembered by noting that the subscripts on the first δ on the RHS are those that immediately follow (cyclically, if necessary) the common subscript, here i, in each ϵ-term on the LHS; the remaining combinations of j, k, l, m as subscripts in the other δ-terms on the RHS can then be filled in automatically.

Contracting (26.35) by setting $j = l$ (say) we obtain, since $\delta_{kk} = 3$ when using the summation convention,

$$\epsilon_{ijk}\epsilon_{ijm} = 3\delta_{km} - \delta_{km} = 2\delta_{km},$$

and by contracting once more, setting $k = m$, we further find that

$$\epsilon_{ijk}\epsilon_{ijk} = 6. \tag{26.36}$$

26.9 Isotropic tensors

It will have been noticed that, unlike most of the tensors discussed (except for scalars), δ_{ij} and ϵ_{ijk} have the property that all their components have values that are the same whatever rotation of axes is made, i.e. the component values

are independent of the transformation L_{ij}. Specifically, δ_{11} has the value 1 in all coordinate frames, whereas for a general second-order tensor **T** all we know is that if $T_{11} = f_{11}(x_1, x_2, x_3)$ then $T'_{11} = f_{11}(x'_1, x'_2, x'_3)$. Tensors with the former property are called *isotropic* (or *invariant*) tensors.

It is important to know the most general form that an isotropic tensor can take, since the description of the physical properties, e.g. the conductivity, magnetic susceptibility or tensile strength, of an isotropic medium (i.e. a medium having the same properties whichever way it is orientated) involves an isotropic tensor. In the previous section it was shown that δ_{ij} and ϵ_{ijk} are second- and third-order isotropic tensors; we will now show that, to within a scalar multiple, they are the only such isotropic tensors.

Let us begin with isotropic second-order tensors. Suppose T_{ij} is an isotropic tensor; then, by definition, for *any* rotation of the axes we must have that

$$T_{ij} = T'_{ij} = L_{ik}L_{jl}T_{kl} \tag{26.37}$$

for each of the nine components.

First consider a rotation of the axes by $2\pi/3$ about the $(1, 1, 1)$ direction; this takes Ox_1, Ox_2, Ox_3 into Ox'_2, Ox'_3, Ox'_1 respectively. For this rotation $L_{13} = 1$, $L_{21} = 1$, $L_{32} = 1$ and all other $L_{ij} = 0$. This requires that $T_{11} = T'_{11} = T_{33}$. Similarly $T_{12} = T'_{12} = T_{31}$. Continuing in this way, we find:

$$\text{(a)}\ T_{11} = T_{22} = T_{33};$$
$$\text{(b)}\ T_{12} = T_{23} = T_{31};$$
$$\text{(c)}\ T_{21} = T_{32} = T_{13}.$$

Next, consider a rotation of the axes (from their original position) by $\pi/2$ about the Ox_3-axis. In this case $L_{12} = -1$, $L_{21} = 1$, $L_{33} = 1$ and all other $L_{ij} = 0$. Amongst other relationships, we must have from (26.37) that:

$$T_{13} = (-1) \times 1 \times T_{23};$$
$$T_{23} = 1 \times 1 \times T_{13}.$$

Hence $T_{13} = T_{23} = 0$ and therefore, by parts (b) and (c) above, each element $T_{ij} = 0$ except for T_{11}, T_{22} and T_{33}, which are all the same. This shows that $T_{ij} = \lambda\delta_{ij}$.

►*Show that $\lambda\epsilon_{ijk}$ is the only isotropic third-order Cartesian tensor.*

The general line of attack is as above and so only a minimum of explanation will be given.

$$T_{ijk} = T'_{ijk} = L_{il}L_{jm}L_{kn}T_{lmn} \quad \text{(in all, there are 27 elements).}$$

Rotate about the $(1, 1, 1)$ direction: this is equivalent to making subscript permutations $1 \to 2 \to 3 \to 1$. We find

(a) $T_{111} = T_{222} = T_{333}$,
(b) $T_{112} = T_{223} = T_{331}$ (and two similar sets),
(c) $T_{123} = T_{231} = T_{312}$ (and a set involving odd permutations of 1, 2, 3).

Rotate by $\pi/2$ about the Ox_3-axis: $L_{12} = -1$, $L_{21} = 1$, $L_{33} = 1$, the other $L_{ij} = 0$.

(d) $T_{111} = (-1) \times (-1) \times (-1) \times T_{222} = -T_{222}$,
(e) $T_{112} = (-1) \times (-1) \times 1 \times T_{221}$,
(f) $T_{221} = 1 \times 1 \times (-1) \times T_{112}$,
(g) $T_{123} = (-1) \times 1 \times 1 \times T_{213}$.

Relations (a) and (d) show that elements with all subscripts the same are zero. Relations (e), (f) and (b) show that all elements with repeated subscripts are zero. Relations (g) and (c) show that $T_{123} = T_{231} = T_{312} = -T_{213} = -T_{321} = -T_{132}$.

In total, T_{ijk} differs from ϵ_{ijk} by at most a scalar factor, but since ϵ_{ijk} (and hence $\lambda\epsilon_{ijk}$) has already been shown to be an isotropic tensor, T_{ijk} must be the most general third-order isotropic Cartesian tensor. ◄

Using exactly the same procedures as those employed for δ_{ij} and ϵ_{ijk}, it may be shown that the only isotropic first-order tensor is the trivial one with all elements zero.

26.10 Improper rotations and pseudotensors

So far we have considered rigid rotations of the coordinate axes described by an orthogonal matrix L with $|\mathsf{L}| = +1$, (26.4). Strictly speaking such transformations are called *proper rotations*. We now broaden our discussion to include transformations that are still described by an orthogonal matrix L but for which $|\mathsf{L}| = -1$; these are called *improper rotations*.

This kind of transformation can always be considered as an *inversion* of the coordinate axes through the origin represented by the equation

$$x_i' = -x_i, \tag{26.38}$$

combined with a proper rotation. The transformation may be looked upon alternatively as one that changes an initially right-handed coordinate system into a left-handed one; any prior or subsequent proper rotation will not change this state of affairs. The most obvious example of a transformation with $|\mathsf{L}| = -1$ is the matrix corresponding to (26.38) itself; in this case $L_{ij} = -\delta_{ij}$.

As we have emphasised in earlier chapters, any real physical vector $\mathbf{v}$ may be considered as a geometrical object (i.e. an arrow in space), which can be referred to independently of any coordinate system and whose direction and magnitude cannot be altered merely by describing it in terms of a different coordinate system. Thus the components of $\mathbf{v}$ transform as $v_i' = L_{ij}v_j$ under *all* rotations (proper and improper).

We can define another type of object, however, whose components may also be labelled by a single subscript but which transforms as $v_i' = L_{ij}v_j$ under proper rotations and as $v_i' = -L_{ij}v_j$ (note the minus sign) under improper rotations. In this case, the v_i are not strictly the components of a true first-order Cartesian tensor but instead are said to form the components of a first-order Cartesian *pseudotensor* or *pseudovector*.

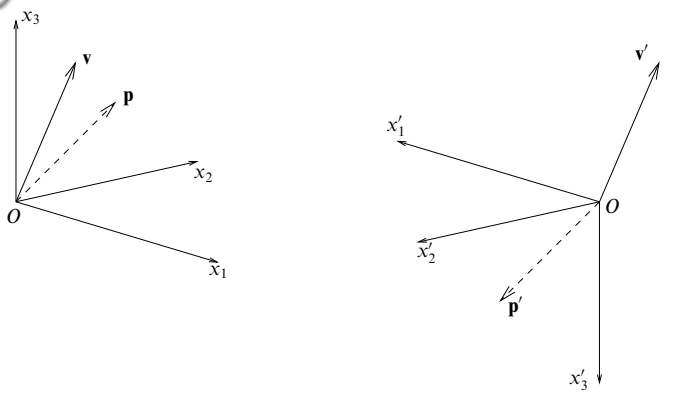


Figure 26.2 The behaviour of a vector **v** and a pseudovector **p** under a reflection through the origin of the coordinate system x_1, x_2, x_3 giving the new system x'_1, x'_2, x'_3.

It is important to realise that a pseudovector (as its name suggests) is not a geometrical object in the usual sense. In particular, it should *not* be considered as a real physical arrow in space, since its direction is reversed by an *improper* transformation of the coordinate axes (such as an inversion through the origin). This is illustrated in figure 26.2, in which the pseudovector **p** is shown as a broken line to indicate that it is not a real physical vector.

Corresponding to vectors and pseudovectors, zeroth-order objects may be divided into scalars and pseudoscalars – the latter being invariant under rotation but changing sign on reflection.

We may also extend the notion of scalars and pseudoscalars, vectors and pseudovectors, to objects with two or more subscripts. For two subcripts, as defined previously, any quantity with components that transform as $T'_{ij} = L_{ik}L_{jl}T_{kl}$ under *all* rotations (proper and improper) is called a second-order Cartesian tensor. If, however, $T'_{ij} = L_{ik}L_{jl}T_{kl}$ under proper rotations but $T'_{ij} = -L_{ik}L_{jl}T_{kl}$ under improper ones (which include reflections), then the T_{ij} are the components of a second-order Cartesian pseudotensor. In general the components of Cartesian pseudotensors of arbitary order transform as

$$T'_{ij\cdots k} = |\mathsf{L}|L_{il}L_{jm}\cdots L_{kn}T_{lm\cdots n}, \tag{26.39}$$

where $|\mathsf{L}|$ is the determinant of the transformation matrix.

For example, from (26.29) we have that

$$|\mathsf{L}|\epsilon_{ijk} = L_{il}L_{jm}L_{kn}\epsilon_{lmn},$$

but since $|\mathsf{L}| = \pm 1$ we may rewrite this as

$$\epsilon_{ijk} = |\mathsf{L}| L_{il} L_{jm} L_{kn} \epsilon_{lmn}.$$

From this expression, we see that although ϵ_{ijk} behaves as a tensor under proper rotations, as discussed in section 26.8, it should properly be regarded as a third-order Cartesian *pseudo*tensor.

► *If b_j and c_k are the components of vectors, show that the quantities $a_i = \epsilon_{ijk} b_j c_k$ form the components of a pseudovector.*

In a new coordinate system we have

$$\begin{aligned} a'_i &= \epsilon'_{ijk} b'_j c'_k \\ &= |\mathsf{L}| L_{il} L_{jm} L_{kn} \epsilon_{lmn} L_{jp} b_p L_{kq} c_q \\ &= |\mathsf{L}| L_{il} \epsilon_{lmn} \delta_{mp} \delta_{nq} b_p c_q \\ &= |\mathsf{L}| L_{il} \epsilon_{lmn} b_m c_n \\ &= |\mathsf{L}| L_{il} a_l, \end{aligned}$$

from which we see immediately that the quantities a_i form the components of a pseudovector. ◄

The above example is worth some further comment. If we denote the vectors with components b_j and c_k by $\mathbf{b}$ and $\mathbf{c}$ respectively then, as mentioned in section 26.8, the quantities $a_i = \epsilon_{ijk} b_j c_k$ are the components of the real vector $\mathbf{a} = \mathbf{b} \times \mathbf{c}$, *provided that we are using a right-handed Cartesian coordinate system.* However, in a coordinate system that is left-handed the quantitites $a'_i = \epsilon'_{ijk} b'_j c'_k$ are *not* the components of the physical vector $\mathbf{a} = \mathbf{b} \times \mathbf{c}$, which has, instead, the components $-a'_i$. It is therefore important to note the handedness of a coordinate system before attempting to write in component form the vector relation $\mathbf{a} = \mathbf{b} \times \mathbf{c}$ (which is true without reference to any coordinate system).

It is worth noting that, although pseudotensors can be useful mathematical objects, the description of the real physical world must usually be in terms of tensors (i.e. scalars, vectors, etc.).[§] For example, the temperature or density of a gas must be a scalar quantity (rather than a pseudoscalar), since its value does not change when the coordinate system used to describe it is inverted through the origin. Similarly, velocity, magnetic field strength or angular momentum can only be described by a vector, and not by a pseudovector.

At this point, it may be useful to make a brief comment on the distinction between *active* and *passive* transformations of a physical system, as this difference often causes confusion. In this chapter, we are concerned solely with passive trans-

[§] In fact the quantum-mechanical description of elementary particles, such as electrons, protons and neutrons, requires the introduction of a new kind of mathematical object called a *spinor*, which is not a scalar, vector, or more general tensor. The study of spinors, however, falls beyond the scope of this book.

formations, for which the physical system of interest is left unaltered, and only the coordinate system used to describe it is changed. In an active transformation, however, the system itself is altered.

As an example, let us consider a particle of mass m that is located at a position $\mathbf{x}$ relative to the origin O and hence has velocity $\dot{\mathbf{x}}$. The angular momentum of the particle about O is thus $\mathbf{J} = m(\mathbf{x} \times \dot{\mathbf{x}})$. If we merely invert the Cartesian coordinates used to describe this system through O, neither the magnitude nor direction of any these vectors will be changed, since they may be considered simply as arrows in space that are independent of the coordinates used to describe them. If, however, we perform the analogous active transformation on the system, by inverting the position vector of the particle through O, then it is clear that the direction of particle's velocity will also be reversed, since it is simply the time derivative of the position vector, but that the direction of its angular momentum vector remains unaltered. This suggests that vectors can be divided into two categories, as follows: *polar* vectors (such as position and velocity), which reverse direction under an active inversion of the physical system through the origin, and *axial* vectors (such as angular momentum), which remain unchanged. It should be emphasised that at no point in this discussion have we used the concept of a pseudovector to describe a real physical quantity.§

26.11 Dual tensors

Although pseudotensors are not themselves appropriate for the description of physical phenomena, they are sometimes needed; for example, we may use the pseudotensor ϵ_{ijk} to associate with every *antisymmetric* second-order tensor A_{ij} (in three dimensions) a pseudovector p_i given by

$$p_i = \tfrac{1}{2}\epsilon_{ijk}A_{jk}; \tag{26.40}$$

p_i is called the *dual* of A_{ij}. Thus if we denote the antisymmetric tensor $\mathbf{A}$ by the matrix

$$\mathsf{A} = [A_{ij}] = \begin{pmatrix} 0 & A_{12} & -A_{31} \\ -A_{12} & 0 & A_{23} \\ A_{31} & -A_{23} & 0 \end{pmatrix}$$

then the components of its dual pseudovector are $(p_1, p_2, p_3) = (A_{23}, A_{31}, A_{12})$.

§ The scalar product of a polar vector and an axial vector is a pseudoscalar. It was the experimental detection of the dependence of the angular distribution of electrons of (polar vector) momentum $\mathbf{p}_e$ emitted by polarised nuclei of (axial vector) spin $\mathbf{J}_N$ upon the pseudoscalar quantity $\mathbf{J}_N \cdot \mathbf{p}_e$ that established the existence of the non-conservation of parity in β-decay.

►*Using (26.40), show that* $A_{ij} = \epsilon_{ijk}p_k$.

By contracting both sides of (26.40) with ϵ_{ijk}, we find

$$\epsilon_{ijk}p_k = \tfrac{1}{2}\epsilon_{ijk}\epsilon_{klm}A_{lm}.$$

Using the identity (26.30) then gives

$$\begin{aligned}\epsilon_{ijk}p_k &= \tfrac{1}{2}(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})A_{lm} \\ &= \tfrac{1}{2}(A_{ij} - A_{ji}) = \tfrac{1}{2}(A_{ij} + A_{ij}) = A_{ij},\end{aligned}$$

where in the last line we use the fact that $A_{ij} = -A_{ji}$. ◄

By a simple extension, we may associate a dual pseudoscalar s with every totally antisymmetric third-rank tensor A_{ijk}, i.e. one that is antisymmetric with respect to the interchange of every possible pair of subscripts; s is given by

$$s = \frac{1}{3!}\epsilon_{ijk}A_{ijk}. \tag{26.41}$$

Since A_{ijk} is a totally antisymmetric three-subscript quantity, we expect it to equal some multiple of ϵ_{ijk} (since this is the only such quantity). In fact $A_{ijk} = s\epsilon_{ijk}$, as can be proved by substituting this expression into (26.41) and using (26.36).

26.12 Physical applications of tensors

In this section some physical applications of tensors will be given. First-order tensors are familiar as vectors and so we will concentrate on second-order tensors, starting with an example taken from mechanics.

Consider a collection of rigidly connected point particles of which the αth, which has mass $m^{(\alpha)}$ and is positioned at $\mathbf{r}^{(\alpha)}$ with respect to an origin O, is typical. Suppose that the rigid assembly is rotating about an axis through O with angular velocity $\boldsymbol{\omega}$.

The angular momentum $\mathbf{J}$ about O of the assembly is given by

$$\mathbf{J} = \sum_{\alpha} \left(\mathbf{r}^{(\alpha)} \times \mathbf{p}^{(\alpha)}\right).$$

But $\mathbf{p}^{(\alpha)} = m^{(\alpha)}\dot{\mathbf{r}}^{(\alpha)}$ and $\dot{\mathbf{r}}^{(\alpha)} = \boldsymbol{\omega} \times \mathbf{r}^{(\alpha)}$, for any α, and so in subscript form the components of $\mathbf{J}$ are given by

$$\begin{aligned}J_i &= \sum_{\alpha} m^{(\alpha)}\epsilon_{ijk}x_j^{(\alpha)}\dot{x}_k^{(\alpha)} \\ &= \sum_{\alpha} m^{(\alpha)}\epsilon_{ijk}x_j^{(\alpha)}\epsilon_{klm}\omega_l x_m^{(\alpha)} \\ &= \sum_{\alpha} m^{(\alpha)}(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})x_j^{(\alpha)}x_m^{(\alpha)}\omega_l \\ &= \sum_{\alpha} m^{(\alpha)}\left[\left(r^{(\alpha)}\right)^2\delta_{il} - x_i^{(\alpha)}x_l^{(\alpha)}\right]\omega_l \equiv I_{il}\omega_l,\end{aligned} \tag{26.42}$$

where I_{il} is a symmetric second-order Cartesian tensor (by the quotient rule, see

section 26.7, since $\mathbf{J}$ and $\boldsymbol{\omega}$ are vectors). The tensor is called the *inertia tensor* at O of the assembly and depends only on the distribution of masses in the assembly and not upon the direction or magnitude of $\boldsymbol{\omega}$.

A more realistic situation obtains if a continuous rigid body is considered. In this case, $m^{(\alpha)}$ must be replaced everywhere by $\rho(\mathbf{r})\,dx\,dy\,dz$ and all summations by integrations over the volume of the body. Written out in full in Cartesians, the inertia tensor for a continuous body would have the form

$$\mathsf{I} = [I_{ij}] = \begin{pmatrix} \int(y^2+z^2)\rho\,dV & -\int xy\rho\,dV & -\int xz\rho\,dV \\ -\int xy\rho\,dV & \int(z^2+x^2)\rho\,dV & -\int yz\rho\,dV \\ -\int xz\rho\,dV & -\int yz\rho\,dV & \int(x^2+y^2)\rho\,dV \end{pmatrix},$$

where $\rho = \rho(x, y, z)$ is the mass distribution and dV stands for $dx\,dy\,dz$; the integrals are to be taken over the whole body. The diagonal elements of this tensor are called the *moments of inertia* and the off-diagonal elements without the minus signs are known as the *products of inertia.*

►*Show that the kinetic energy of the rotating system is given by* $T = \frac{1}{2}I_{jl}\omega_j\omega_l$.

By an argument parallel to that already made for $\mathbf{J}$, the kinetic energy is given by

$$\begin{aligned} T &= \tfrac{1}{2}\sum_\alpha m^{(\alpha)}\left(\dot{\mathbf{r}}^{(\alpha)}\cdot\dot{\mathbf{r}}^{(\alpha)}\right) \\ &= \tfrac{1}{2}\sum_\alpha m^{(\alpha)}\epsilon_{ijk}\omega_j x_k^{(\alpha)}\epsilon_{ilm}\omega_l x_m^{(\alpha)} \\ &= \tfrac{1}{2}\sum_\alpha m^{(\alpha)}(\delta_{jl}\delta_{km}-\delta_{jm}\delta_{kl})x_k^{(\alpha)}x_m^{(\alpha)}\omega_j\omega_l \\ &= \tfrac{1}{2}\sum_\alpha m^{(\alpha)}\left[\delta_{jl}\left(r^{(\alpha)}\right)^2 - x_j^{(\alpha)}x_l^{(\alpha)}\right]\omega_j\omega_l \\ &= \tfrac{1}{2}I_{jl}\omega_j\omega_l. \end{aligned}$$

Alternatively, since $J_j = I_{jl}\omega_l$ we may write the kinetic energy of the rotating system as $T = \frac{1}{2}J_j\omega_j$. ◄

The above example shows that the kinetic energy of the rotating body can be expressed as a scalar obtained by twice contracting $\boldsymbol{\omega}$ with the inertia tensor. It also shows that the moment of inertia of the body about a line given by the unit vector $\hat{\mathbf{n}}$ is $I_{jl}\hat{n}_j\hat{n}_l$ (or $\hat{\mathsf{n}}^{\mathrm{T}}\mathsf{I}\hat{\mathsf{n}}$ in matrix form).

Since $\mathbf{I}$ ($\equiv I_{jl}$) is a real symmetric second-order tensor, it has associated with it three mutually perpendicular directions that are its *principal axes* and have the following properties (proved in chapter 8):

(i) with each axis is associated a principal moment of inertia λ_μ, $\mu = 1, 2, 3$;

(ii) when the rotation of the body is about one of these axes, the angular velocity and the angular momentum are parallel and given by

$$\mathbf{J} = \mathbf{I}\boldsymbol{\omega} = \lambda_\mu\boldsymbol{\omega},$$

i.e. $\boldsymbol{\omega}$ is an eigenvector of $\mathbf{I}$ with eigenvalue λ_μ;

(iii) referred to these axes as coordinate axes, the inertia tensor is diagonal with diagonal entries $\lambda_1, \lambda_2, \lambda_3$.

Two further examples of physical quantities represented by second-order tensors are magnetic susceptibility and electrical conductivity. In the first case we have (in standard notation)

$$M_i = \chi_{ij} H_j, \tag{26.43}$$

and in the second case

$$j_i = \sigma_{ij} E_j. \tag{26.44}$$

Here $\mathbf{M}$ is the magnetic moment per unit volume and $\mathbf{j}$ the current density (current per unit perpendicular area). In both cases we have on the left-hand side a vector and on the right-hand side the contraction of a set of quantities with another vector. Each set of quantities must therefore form the components of a second-order tensor.

For isotropic media $\mathbf{M} \propto \mathbf{H}$ and $\mathbf{j} \propto \mathbf{E}$, but for anisotropic materials such as crystals the susceptibility and conductivity may be different along different crystal axes, making χ_{ij} and σ_{ij} general second-order tensors, although they are usually symmetric.

► *The electrical conductivity $\boldsymbol{\sigma}$ in a crystal is measured by an observer to have components as shown:*

$$[\sigma_{ij}] = \begin{pmatrix} 1 & \sqrt{2} & 0 \\ \sqrt{2} & 3 & 1 \\ 0 & 1 & 1 \end{pmatrix}. \tag{26.45}$$

Show that there is one direction in the crystal along which no current can flow. Does the current flow equally easily in the two perpendicular directions?

The current density in the crystal is given by $j_i = \sigma_{ij} E_j$, where σ_{ij}, relative to the observer's coordinate system, is given by (26.45). Since $[\sigma_{ij}]$ is a symmetric matrix, it possesses three mutually perpendicular eigenvectors (or principal axes) with respect to which the conductivity tensor is diagonal, with diagonal entries $\lambda_1, \lambda_2, \lambda_3$, the eigenvalues of $[\sigma_{ij}]$.

As discussed in chapter 8, the eigenvalues of $[\sigma_{ij}]$ are given by $|\sigma - \lambda \mathbf{I}| = 0$. Thus we require

$$\begin{vmatrix} 1-\lambda & \sqrt{2} & 0 \\ \sqrt{2} & 3-\lambda & 1 \\ 0 & 1 & 1-\lambda \end{vmatrix} = 0,$$

from which we find

$$(1-\lambda)[(3-\lambda)(1-\lambda) - 1] - 2(1-\lambda) = 0.$$

This simplifies to give $\lambda = 0, 1, 4$ so that, with respect to its principal axes, the conductivity tensor has components σ'_{ij} given by

$$[\sigma'_{ij}] = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Since $j'_i = \sigma'_{ij} E'_j$, we see immediately that along one of the principal axes there is no current flow and along the two perpendicular directions the current flows are not equal. ◄

We can extend the idea of a second-order tensor that relates two vectors to a situation where two physical second-order tensors are related by a fourth-order tensor. The most common occurrence of such relationships is in the theory of elasticity. This is not the place to give a detailed account of elasticity theory, but suffice it to say that the local deformation of an elastic body at any interior point P can be described by a second-order symmetric tensor e_{ij} called the *strain tensor*. It is given by

$$e_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right),$$

where $\mathbf{u}$ is the displacement vector describing the strain of a small volume element whose unstrained position relative to the origin is $\mathbf{x}$. Similarly we can describe the stress in the body at P by the second-order symmetric *stress tensor* p_{ij}; the quantity p_{ij} is the x_j-component of the stress vector acting across a plane through P whose normal lies in the x_i-direction. A generalisation of Hooke's law then relates the stress and strain tensors by

$$p_{ij} = c_{ijkl}e_{kl} \tag{26.46}$$

where c_{ijkl} is a fourth-order Cartesian tensor.

►*Assuming that the most general fourth-order isotropic tensor is*

$$c_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \eta\delta_{ik}\delta_{jl} + \nu\delta_{il}\delta_{jk}, \tag{26.47}$$

find the form of (26.46) for an isotropic medium having Young's modulus E and Poisson's ratio σ.

For an isotropic medium we must have an isotropic tensor for c_{ijkl}, and so we assume the form (26.47). Substituting this into (26.46) yields

$$p_{ij} = \lambda\delta_{ij}e_{kk} + \eta e_{ij} + \nu e_{ji}.$$

But e_{ij} is symmetric, and if we write $\eta + \nu = 2\mu$, then this takes the form

$$p_{ij} = \lambda e_{kk}\delta_{ij} + 2\mu e_{ij},$$

in which λ and μ are known as *Lamé constants*. It will be noted that if $e_{ij} = 0$ for $i \neq j$ then the same is true of p_{ij}, i.e. the principal axes of the stress and strain tensors coincide.

Now consider a simple tension in the x_1-direction, i.e. $p_{11} = S$ but all other $p_{ij} = 0$. Then denoting e_{kk} (summed over k) by θ we have, in addition to $e_{ij} = 0$ for $i \neq j$, the three equations

$$\begin{aligned} S &= \lambda\theta + 2\mu e_{11}, \\ 0 &= \lambda\theta + 2\mu e_{22}, \\ 0 &= \lambda\theta + 2\mu e_{33}. \end{aligned}$$

Adding them gives

$$S = \theta(3\lambda + 2\mu).$$

Substituting for θ from this into the first of the three, and recalling that Young's modulus is defined by $S = Ee_{11}$, gives E as

$$E = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu}. \tag{26.48}$$

Further, Poisson's ratio is defined as $\sigma = -e_{22}/e_{11}$ (or $-e_{33}/e_{11}$) and is thus

$$\sigma = \left(\frac{1}{e_{11}}\right)\frac{\lambda\theta}{2\mu} = \left(\frac{1}{e_{11}}\right)\left(\frac{\lambda}{2\mu}\right)\frac{Ee_{11}}{3\lambda+2\mu} = \frac{\lambda}{2(\lambda+\mu)}. \tag{26.49}$$

Solving (26.48) and (26.49) for λ and μ gives finally

$$p_{ij} = \frac{\sigma E}{(1+\sigma)(1-2\sigma)}e_{kk}\delta_{ij} + \frac{E}{(1+\sigma)}e_{ij}. \blacktriangleleft$$

26.13 Integral theorems for tensors

In chapter 11, we discussed various integral theorems involving vector and scalar fields. Most notably, we considered the divergence theorem, which states that, for any vector field **a**,

$$\int_V \nabla\cdot\mathbf{a}\,dV = \oint_S \mathbf{a}\cdot\hat{\mathbf{n}}\,dS, \tag{26.50}$$

where S is the surface enclosing the volume V and $\hat{\mathbf{n}}$ is the outward-pointing unit normal to S at each point.

Writing (26.50) in subscript notation, we have

$$\int_V \frac{\partial a_k}{\partial x_k}\,dV = \oint_S a_k\hat{n}_k\,dS. \tag{26.51}$$

Although we shall not prove it rigorously, (26.51) can be extended in an obvious manner to relate integrals of *tensor fields*, rather than just vector fields, over volumes and surfaces, with the result

$$\int_V \frac{\partial T_{ij\ldots k\ldots m}}{\partial x_k}\,dV = \oint_S T_{ij\ldots k\ldots m}\hat{n}_k\,dS.$$

This form of the divergence theorem for general tensors can be very useful in vector calculus manipulations.

►*A vector field* **a** *satisfies* $\nabla\cdot\mathbf{a} = 0$ *inside some volume* V *and* $\mathbf{a}\cdot\hat{\mathbf{n}} = 0$ *on the boundary surface* S. *By considering the divergence theorem applied to* $T_{ij} = x_i a_j$, *show that* $\int_V \mathbf{a}\,dV = \mathbf{0}$.

Applying the divergence theorem to $T_{ij} = x_i a_j$ we find

$$\int_V \frac{\partial T_{ij}}{\partial x_j}\,dV = \int_V \frac{\partial(x_i a_j)}{\partial x_j}\,dV = \oint_S x_i a_j\hat{n}_j\,dS = 0,$$

since $a_j\hat{n}_j = 0$. By expanding the volume integral we obtain

$$\begin{aligned}\int_V \frac{\partial(x_i a_j)}{\partial x_j}\,dV &= \int_V \frac{\partial x_i}{\partial x_j}a_j\,dV + \int_V x_i\frac{\partial a_j}{\partial x_j}\,dV\\ &= \int_V \delta_{ij}a_j\,dV\\ &= \int_V a_i\,dV = 0,\end{aligned}$$

where in going from the first to the second line we used $\partial x_i/\partial x_j = \delta_{ij}$ and $\partial a_j/\partial x_j = 0$. ◄

The other integral theorems discussed in chapter 11 can be extended in a similar way. For example, written in tensor notation Stokes' theorem states that, for a vector field a_i,

$$\int_S \epsilon_{ijk} \frac{\partial a_k}{\partial x_j} \hat{n}_i \, dS = \oint_C a_k \, dx_k.$$

For a general tensor field this has the straightforward extension

$$\int_S \epsilon_{ijk} \frac{\partial T_{lm\cdots k\cdots n}}{\partial x_j} \hat{n}_i \, dS = \oint_C T_{lm\cdots k\cdots n} \, dx_k.$$

26.14 Non-Cartesian coordinates

So far we have restricted our attention to the study of tensors when they are described in terms of Cartesian coordinates and the axes of coordinates are rigidly rotated, sometimes together with an inversion of axes through the origin. In the remainder of this chapter we shall extend the concepts discussed in the previous sections by considering arbitrary coordinate transformations from one general coordinate system to another. Although this generalisation brings with it several complications, we shall find that many of the properties of Cartesian tensors are still valid for more general tensors. Before considering general coordinate transformations, however, we begin by reminding ourselves of some properties of general curvilinear coordinates, as discussed in chapter 10.

The position of an arbitrary point P in space may be expressed in terms of the three curvilinear coordinates u_1, u_2, u_3. We saw in chapter 10 that if $\mathbf{r}(u_1, u_2, u_3)$ is the position vector of the point P then at P there exist two sets of basis vectors

$$\mathbf{e}_i = \frac{\partial \mathbf{r}}{\partial u_i} \qquad \text{and} \qquad \boldsymbol{\epsilon}_i = \nabla u_i, \tag{26.52}$$

where $i = 1, 2, 3$. In general, the vectors in each set neither are of unit length nor form an orthogonal basis. However, the sets $\mathbf{e}_i$ and $\boldsymbol{\epsilon}_i$ are reciprocal systems of vectors and so

$$\mathbf{e}_i \cdot \boldsymbol{\epsilon}_j = \delta_{ij}. \tag{26.53}$$

In the context of general tensor analysis, it is more usual to denote the second set of vectors $\boldsymbol{\epsilon}_i$ in (26.52) by $\mathbf{e}^i$, the index being placed as a superscript to distinguish it from the (different) vector $\mathbf{e}_i$, which is a member of the first set in (26.52). Although this positioning of the index may seem odd (not least because of the possibility of confusion with powers) it forms part of a slight modification to the summation convention that we will adopt for the remainder of this chapter. This is as follows: any lower-case alphabetic index that appears exactly twice in any term of an expression, *once as a subscript and once as a superscript*, is to be summed over all the values that an index in that position can take (unless the

contrary is specifically stated). All other aspects of the summation convention remain unchanged.

With the introduction of superscripts, the reciprocity relation (26.53) should be rewritten so that both sides of (26.54) have one subscript and one superscript, i.e. as

$$\mathbf{e}_i \cdot \mathbf{e}^j = \delta_i^j. \tag{26.54}$$

The alternative form of the Kronecker delta is defined in a similar way to previously, i.e. it equals unity if $i = j$ and is zero otherwise.

For similar reasons it is usual to denote the curvilinear coordinates themselves by u^1, u^2, u^3, with the index raised, so that

$$\mathbf{e}_i = \frac{\partial \mathbf{r}}{\partial u^i} \qquad \text{and} \qquad \mathbf{e}^i = \nabla u^i. \tag{26.55}$$

From the first equality we see that we may consider a superscript that appears in the denominator of a partial derivative as a subscript.

Given the two bases $\mathbf{e}_i$ and $\mathbf{e}^i$, we may write a general vector $\mathbf{a}$ equally well in terms of either basis as follows:

$$\mathbf{a} = a^1\mathbf{e}_1 + a^2\mathbf{e}_2 + a^3\mathbf{e}_3 = a^i\mathbf{e}_i;$$
$$\mathbf{a} = a_1\mathbf{e}^1 + a_2\mathbf{e}^2 + a_3\mathbf{e}^3 = a_i\mathbf{e}^i.$$

The a^i are called the *contravariant* components of the vector $\mathbf{a}$ and the a_i the *covariant* components, the position of the index (either as a subscript or superscript) serving to distinguish between them. Similarly, we may call the $\mathbf{e}_i$ the covariant basis vectors and the $\mathbf{e}^i$ the contravariant ones.

►*Show that the contravariant and covariant components of a vector* $\mathbf{a}$ *are given by* $a^i = \mathbf{a}\cdot\mathbf{e}^i$ *and* $a_i = \mathbf{a}\cdot\mathbf{e}_i$ *respectively.*

For the contravariant components, we find

$$\mathbf{a}\cdot\mathbf{e}^i = a^j\mathbf{e}_j\cdot\mathbf{e}^i = a^j\delta_j^i = a^i,$$

where we have used the reciprocity relation (26.54). Similarly, for the covariant components,

$$\mathbf{a}\cdot\mathbf{e}_i = a_j\mathbf{e}^j\cdot\mathbf{e}_i = a_j\delta_i^j = a_i. \blacktriangleleft$$

The reason that the notion of contravariant and covariant components of a vector (and the resulting superscript notation) was not introduced earlier is that for Cartesian coordinate systems the two sets of basis vectors $\mathbf{e}_i$ and $\mathbf{e}^i$ are identical and, hence, so are the components of a vector with respect to either basis. Thus, for Cartesian coordinates, we may speak simply of the components of the vector and there is no need to differentiate between contravariance and covariance, or to introduce superscripts to make a distinction between them.

If we consider the components of higher-order tensors in non-Cartesian coordinates, there are even more possibilities. As an example, let us consider a

second-order tensor $\mathbf{T}$. Using the outer product notation in (26.23), we may write $\mathbf{T}$ in three different ways:

$$\mathbf{T} = T^{ij}\mathbf{e}_i \otimes \mathbf{e}_j = T^i{}_j\mathbf{e}_i \otimes \mathbf{e}^j = T_{ij}\mathbf{e}^i \otimes \mathbf{e}^j,$$

where T^{ij}, $T^i{}_j$ and T_{ij} are called the *contravariant, mixed* and *covariant* components of $\mathbf{T}$ respectively. It is important to remember that these three sets of quantities form the components of the *same* tensor $\mathbf{T}$ but refer to different (tensor) bases made up from the basis vectors of the coordinate system. Again, if we are using Cartesian coordinates then all three sets of components are identical.

We may generalise the above equation to higher-order tensors. Components carrying only superscripts or only subscripts are referred to as the contravariant and covariant components respectively; all others are called mixed components.

26.15 The metric tensor

Any particular curvilinear coordinate system is completely characterised at each point in space by the nine quantities

$$g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j, \tag{26.56}$$

which, as we will show, are the covariant components of a symmetric second-order tensor $\mathbf{g}$ called the *metric tensor*.

Since an infinitesimal vector displacement can be written as $d\mathbf{r} = du^i\mathbf{e}_i$, we find that the square of the infinitesimal arc length $(ds)^2$ can be written in terms of the metric tensor as

$$(ds)^2 = d\mathbf{r} \cdot d\mathbf{r} = du^i\mathbf{e}_i \cdot du^j\mathbf{e}_j = g_{ij}\,du^i du^j. \tag{26.57}$$

It may further be shown that the volume element dV is given by

$$dV = \sqrt{g}\,du^1\,du^2\,du^3, \tag{26.58}$$

where g is the determinant of the matrix $[g_{ij}]$, which has the covariant components of the metric tensor as its elements.

If we compare equations (26.57) and (26.58) with the analogous ones in section 10.10 then we see that in the special case where the coordinate system is orthogonal (so that $\mathbf{e}_i \cdot \mathbf{e}_j = 0$ for $i \neq j$) the metric tensor can be written in terms of the coordinate-system scale factors h_i, $i = 1, 2, 3$ as

$$g_{ij} = \begin{cases} h_i^2 & i = j, \\ 0 & i \neq j. \end{cases}$$

Its determinant is then given by $g = h_1^2h_2^2h_3^2$.

►*Calculate the elements g_{ij} of the metric tensor for cylindrical polar coordinates. Hence find the square of the infinitesimal arc length $(ds)^2$ and the volume dV for this coordinate system.*

As discussed in section 10.9, in cylindrical polar coordinates $(u^1, u^2, u^3) = (\rho, \phi, z)$ and so the position vector $\mathbf{r}$ of any point P may be written

$$\mathbf{r} = \rho\cos\phi\ \mathbf{i} + \rho\sin\phi\ \mathbf{j} + z\,\mathbf{k}.$$

From this we obtain the (covariant) basis vectors:

$$\begin{aligned}\mathbf{e}_1 &= \frac{\partial\mathbf{r}}{\partial\rho} = \cos\phi\ \mathbf{i} + \sin\phi\ \mathbf{j};\\ \mathbf{e}_2 &= \frac{\partial\mathbf{r}}{\partial\phi} = -\rho\sin\phi\ \mathbf{i} + \rho\cos\phi\ \mathbf{j};\\ \mathbf{e}_3 &= \frac{\partial\mathbf{r}}{\partial z} = \mathbf{k}.\end{aligned} \tag{26.59}$$

Thus the components of the metric tensor $[g_{ij}] = [\mathbf{e}_i \cdot \mathbf{e}_j]$ are found to be

$$\mathsf{G} = [g_{ij}] = \begin{pmatrix} 1 & 0 & 0\\ 0 & \rho^2 & 0\\ 0 & 0 & 1\end{pmatrix}, \tag{26.60}$$

from which we see that, as expected for an orthogonal coordinate system, the metric tensor is diagonal, the diagonal elements being equal to the squares of the scale factors of the coordinate system.

From (26.57), the square of the infinitesimal arc length in this coordinate system is given by

$$(ds)^2 = g_{ij}\,du^i\,du^j = (d\rho)^2 + \rho^2(d\phi)^2 + (dz)^2,$$

and, using (26.58), the volume element is found to be

$$dV = \sqrt{g}\,du^1\,du^2\,du^3 = \rho\,d\rho\,d\phi\,dz.$$

These expressions are identical to those derived in section 10.9. ◄

We may also express the scalar product of two vectors in terms of the metric tensor:

$$\mathbf{a}\cdot\mathbf{b} = a^i\mathbf{e}_i \cdot b^j\mathbf{e}_j = g_{ij}a^i b^j, \tag{26.61}$$

where we have used the contravariant components of the two vectors. Similarly, using the covariant components, we can write the same scalar product as

$$\mathbf{a}\cdot\mathbf{b} = a_i\mathbf{e}^i \cdot b_j\mathbf{e}^j = g^{ij}a_i b_j, \tag{26.62}$$

where we have defined the nine quantities $g^{ij} = \mathbf{e}^i\cdot\mathbf{e}^j$. As we shall show, they form the contravariant components of the metric tensor $\mathbf{g}$ and are, in general, different from the quantities g_{ij}. Finally, we could express the scalar product in terms of the contravariant components of one vector and the covariant components of the other,

$$\mathbf{a}\cdot\mathbf{b} = a_i\mathbf{e}^i \cdot b^j\mathbf{e}_j = a_i b^j\delta^i_j = a_i b^i, \tag{26.63}$$

where we have used the reciprocity relation (26.54). Similarly, we could write

$$\mathbf{a} \cdot \mathbf{b} = a^i \mathbf{e}_i \cdot b_j \mathbf{e}^j = a^i b_j \delta_i^j = a^i b_i. \tag{26.64}$$

By comparing the four alternative expressions (26.61)–(26.64) for the scalar product of two vectors we can deduce one of the most useful properties of the quantities g_{ij} and g^{ij}. Since $g_{ij} a^i b^j = a^i b_i$ holds for any arbitrary vector components a^i, it follows that

$$g_{ij} b^j = b_i,$$

which illustrates the fact that the covariant components g_{ij} of the metric tensor can be used to *lower an index*. In other words, it provides a means of obtaining the covariant components of a vector from its contravariant components. By a similar argument, we have

$$g^{ij} b_j = b^i,$$

so that the contravariant components g^{ij} can be used to perform the reverse operation of *raising an index*.

It is straightforward to show that the contravariant and covariant basis vectors, $\mathbf{e}^i$ and $\mathbf{e}_i$ respectively, are related in the same way as other vectors, i.e. by

$$\mathbf{e}^i = g^{ij} \mathbf{e}_j \qquad \text{and} \qquad \mathbf{e}_i = g_{ij} \mathbf{e}^j.$$

We also note that, since $\mathbf{e}_i$ and $\mathbf{e}^i$ are reciprocal systems of vectors in three-dimensional space (see chapter 7), we may write

$$\mathbf{e}^i = \frac{\mathbf{e}_j \times \mathbf{e}_k}{\mathbf{e}_i \cdot (\mathbf{e}_j \times \mathbf{e}_k)},$$

for the combination of subscripts $i, j, k = 1, 2, 3$ and its cyclic permutations. A similar expression holds for $\mathbf{e}_i$ in terms of the $\mathbf{e}^i$-basis. Moreover, it may be shown that $|\mathbf{e}_1 \cdot (\mathbf{e}_2 \times \mathbf{e}_3)| = \sqrt{g}$.

►*Show that the matrix* $[g^{ij}]$ *is the inverse of the matrix* $[g_{ij}]$. *Hence calculate the contravariant components* g^{ij} *of the metric tensor in cylindrical polar coordinates.*

Using the index-lowering and index-raising properties of g_{ij} and g^{ij} on an arbitrary vector $\mathbf{a}$, we find

$$\delta_k^i a^k = a^i = g^{ij} a_j = g^{ij} g_{jk} a^k.$$

But, since $\mathbf{a}$ is arbitrary, we must have

$$g^{ij} g_{jk} = \delta_k^i. \tag{26.65}$$

Denoting the matrix $[g_{ij}]$ by G and $[g^{ij}]$ by $\hat{\mathsf{G}}$, equation (26.65) can be written in matrix form as $\hat{\mathsf{G}}\mathsf{G} = \mathsf{I}$, where I is the unit matrix. Hence G and $\hat{\mathsf{G}}$ are inverse matrices of each other.

Thus, by inverting the matrix G in (26.60), we find that the elements g^{ij} are given in cylindrical polar coordinates by

$$\hat{\mathsf{G}} = [g^{ij}] = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/\rho^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \blacktriangleleft$$

So far we have not considered the components of the metric tensor g^i_j with one subscript and one superscript. By analogy with (26.56), these mixed components are given by

$$g^i_j = \mathbf{e}^i \cdot \mathbf{e}_j = \delta^i_j,$$

and so the components of g^i_j are identical to those of δ^i_j. We may therefore consider the δ^i_j to be the mixed components of the metric tensor $\mathbf{g}$.

26.16 General coordinate transformations and tensors

We now discuss the concept of general transformations from one coordinate system, u^1, u^2, u^3, to another, u'^1, u'^2, u'^3. We can describe the coordinate transform using the three equations

$$u'^i = u'^i(u^1, u^2, u^3),$$

for $i = 1, 2, 3$, in which the new coordinates u'^i can be arbitrary functions of the old ones u^i rather than just represent linear orthogonal transformations (rotations) of the coordinate axes. We shall assume also that the transformation can be inverted, so that we can write the old coordinates in terms of the new ones as

$$u^i = u^i(u'^1, u'^2, u'^3),$$

As an example, we may consider the transformation from spherical polar to Cartesian coordinates, given by

$$\begin{aligned} x &= r \sin\theta \cos\phi, \\ y &= r \sin\theta \sin\phi, \\ z &= r \cos\theta, \end{aligned}$$

which is clearly not a linear transformation.

The two sets of basis vectors in the new coordinate system, u'^1, u'^2, u'^3, are given as in (26.55) by

$$\mathbf{e}'_i = \frac{\partial \mathbf{r}}{\partial u'^i} \qquad \text{and} \qquad \mathbf{e}'^i = \nabla u'^i. \tag{26.66}$$

Considering the first set, we have from the chain rule that

$$\frac{\partial \mathbf{r}}{\partial u^j} = \frac{\partial u'^i}{\partial u^j} \frac{\partial \mathbf{r}}{\partial u'^i},$$

so that the basis vectors in the old and new coordinate systems are related by

$$\mathbf{e}_j = \frac{\partial u'^i}{\partial u^j}\mathbf{e}'_i. \tag{26.67}$$

Now, since we can write any arbitrary vector $\mathbf{a}$ in terms of either basis as

$$\mathbf{a} = a'^i\mathbf{e}'_i = a^j\mathbf{e}_j = a^j\frac{\partial u'^i}{\partial u^j}\mathbf{e}'_i,$$

it follows that the contravariant components of a vector must transform as

$$a'^i = \frac{\partial u'^i}{\partial u^j}a^j. \tag{26.68}$$

In fact, we use this relation as the defining property for a set of quantities a^i to form the contravariant components of a vector.

►*Find an expression analogous to (26.67) relating the basis vectors* $\mathbf{e}^i$ *and* $\mathbf{e}'^i$ *in the two coordinate systems. Hence deduce the way in which the covariant components of a vector change under a coordinate transformation.*

If we consider the second set of basis vectors in (26.66), $\mathbf{e}'^i = \nabla u'^i$, we have from the chain rule that

$$\frac{\partial u^j}{\partial x} = \frac{\partial u^j}{\partial u'^i}\frac{\partial u'^i}{\partial x}$$

and similarly for $\partial u^j/\partial y$ and $\partial u^j/\partial z$. So the basis vectors in the old and new coordinate systems are related by

$$\mathbf{e}^j = \frac{\partial u^j}{\partial u'^i}\mathbf{e}'^i. \tag{26.69}$$

For any arbitrary vector $\mathbf{a}$,

$$\mathbf{a} = a'_i\mathbf{e}'^i = a_j\mathbf{e}^j = a_j\frac{\partial u^j}{\partial u'^i}\mathbf{e}'^i$$

and so the covariant components of a vector must transform as

$$a'_i = \frac{\partial u^j}{\partial u'^i}a_j. \tag{26.70}$$

Analogously to the contravariant case (26.68), we take this result as the defining property of the covariant components of a vector. ◄

We may compare the transformation laws (26.68) and (26.70) with those for a first-order Cartesian tensor under a rigid rotation of axes. Let us consider a rotation of Cartesian axes x^i through an angle θ about the 3-axis to a new set x'^i, $i = 1, 2, 3$, as given by (26.7) and the inverse transformation (26.8). It is straightforward to show that

$$\frac{\partial x^j}{\partial x'^i} = \frac{\partial x'^i}{\partial x^j} = L_{ij},$$

where the elements L_{ij} are given by

$$\mathsf{L} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Thus (26.68) and (26.70) agree with our earlier definition in the special case of a rigid rotation of Cartesian axes.

Following on from (26.68) and (26.70), we proceed in a similar way to define general tensors of higher rank. For example, the contravariant, mixed and covariant components, respectively, of a second-order tensor must transform as follows:

$$\text{contravariant components,} \qquad T'^{ij} = \frac{\partial u'^i}{\partial u^k}\frac{\partial u'^j}{\partial u^l}T^{kl} \ ;$$

$$\text{mixed components,} \qquad T'^i{}_j = \frac{\partial u'^i}{\partial u^k}\frac{\partial u^l}{\partial u'^j}T^k{}_l \ ;$$

$$\text{covariant components,} \qquad T'_{ij} = \frac{\partial u^k}{\partial u'^i}\frac{\partial u^l}{\partial u'^j}T_{kl}.$$

It is important to remember that these quantities form the components of the *same* tensor **T** but refer to different tensor bases made up from the basis vectors of the different coordinate systems. For example, in terms of the contravariant components we may write

$$\mathbf{T} = T^{ij}\mathbf{e}_i \otimes \mathbf{e}_j = T'^{ij}\mathbf{e}'_i \otimes \mathbf{e}'_j.$$

We can clearly go on to define tensors of higher order, with arbitrary numbers of covariant (subscript) and contravariant (superscript) indices, by demanding that their components transform as follows:

$$T'^{ij\cdots k}{}_{lm\cdots n} = \frac{\partial u'^i}{\partial u^a}\frac{\partial u'^j}{\partial u^b}\cdots\frac{\partial u'^k}{\partial u^c}\frac{\partial u^d}{\partial u'^l}\frac{\partial u^e}{\partial u'^m}\cdots\frac{\partial u^f}{\partial u'^n}T^{ab\cdots c}{}_{de\cdots f}. \tag{26.71}$$

Using the revised summation convention described in section 26.14, the algebra of general tensors is completely analogous to that of the Cartesian tensors discussed earlier. For example, as with Cartesian coordinates, the Kronecker delta is a tensor provided it is written as the mixed tensor δ^i_j since

$$\delta'^i{}_j = \frac{\partial u'^i}{\partial u^k}\frac{\partial u^l}{\partial u'^j}\delta^k_l = \frac{\partial u'^i}{\partial u^k}\frac{\partial u^k}{\partial u'^j} = \frac{\partial u'^i}{\partial u'^j} = \delta^i_j,$$

where we have used the chain rule to justify the third equality. This also shows that δ^i_j is isotropic. As discussed at the end of section 26.15, the δ^i_j can be considered as the mixed components of the metric tensor **g**.

►*Show that the quantities* $g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$ *form the covariant components of a second-order tensor.*

In the new (primed) coordinate system we have

$$g'_{ij} = \mathbf{e}'_i \cdot \mathbf{e}'_j,$$

but using (26.67) for the inverse transformation, we have

$$\mathbf{e}'_i = \frac{\partial u^k}{\partial u'^i}\mathbf{e}_k,$$

and similarly for $\mathbf{e}'_j$. Thus we may write

$$g'_{ij} = \frac{\partial u^k}{\partial u'^i}\frac{\partial u^l}{\partial u'^j}\,\mathbf{e}_k \cdot \mathbf{e}_l = \frac{\partial u^k}{\partial u'^i}\frac{\partial u^l}{\partial u'^j}g_{kl},$$

which shows that the g_{ij} are indeed the covariant components of a second-order tensor (the metric tensor $\mathbf{g}$). ◄

A similar argument to that used in the above example shows that the quantities g^{ij} form the contravariant components of a second-order tensor which transforms according to

$$g'^{ij} = \frac{\partial u'^i}{\partial u^k}\frac{\partial u'^j}{\partial u^l}g^{kl}.$$

In the previous section we discussed the use of the components g_{ij} and g^{ij} in the raising and lowering of indices in contravariant and covariant vectors. This can be extended to tensors of arbitrary rank. In general, contraction of a tensor with g_{ij} will convert the contracted index from being contravariant (superscript) to covariant (subscript), i.e. it is lowered. This can be repeated for as many indices are required. For example,

$$T_{ij} = g_{ik}T^k{}_j = g_{ik}g_{jl}T^{kl}. \tag{26.72}$$

Similarly contraction with g^{ij} raises an index, i.e.

$$T^{ij} = g^{ik}T_k{}^j = g^{ik}g^{jl}T_{kl}. \tag{26.73}$$

That (26.72) and (26.73) are mutually consistent may be shown by using the fact that $g^{ik}g_{kj} = \delta^i_j$.

26.17 Relative tensors

In section 26.10 we introduced the concept of pseudotensors in the context of the rotation (proper or improper) of a set of Cartesian axes. Generalising to arbitrary coordinate transformations leads to the notion of a *relative tensor*.

For an arbitrary coordinate transformation from one general coordinate system

u^i to another u'^i, we may define the Jacobian of the transformation (see chapter 6) as the determinant of the transformation matrix $[\partial u'^i/\partial u^j]$: this is usually denoted by

$$J = \left|\frac{\partial u'}{\partial u}\right|.$$

Alternatively, we may interchange the primed and unprimed coordinates to obtain $|\partial u/\partial u'| = 1/J$: unfortunately this also is often called the Jacobian of the transformation.

Using the Jacobian J, we define a relative tensor of weight w as one whose components transform as follows:

$$T'^{ij\cdots k}{}_{lm\cdots n} = \frac{\partial u'^i}{\partial u^a}\frac{\partial u'^j}{\partial u^b}\cdots\frac{\partial u'^k}{\partial u^c}\frac{\partial u^d}{\partial u'^l}\frac{\partial u^e}{\partial u'^m}\cdots\frac{\partial u^f}{\partial u'^n}T^{ab\cdots c}{}_{de\cdots f}\left|\frac{\partial u}{\partial u'}\right|^w. \tag{26.74}$$

Comparing this expression with (26.71), we see that a true (or *absolute*) general tensor may be considered as a relative tensor of weight $w = 0$. If $w = -1$, on the other hand, the relative tensor is known as a general *pseudotensor* and if $w = 1$ as a *tensor density*.

It is worth comparing (26.74) with the definition (26.39) of a Cartesian pseudotensor. For the latter, we are concerned only with its behaviour under a rotation (proper or improper) of Cartesian axes, for which the Jacobian $J = \pm 1$. Thus, general relative tensors of weight $w = -1$ and $w = 1$ would both satisfy the definition (26.39) of a Cartesian pseudotensor.

►*If the g_{ij} are the covariant components of the metric tensor, show that the determinant g of the matrix $[g_{ij}]$ is a relative scalar of weight $w = 2$.*

The components g_{ij} transform as

$$g'_{ij} = \frac{\partial u^k}{\partial u'^i}\frac{\partial u^l}{\partial u'^j}g_{kl}.$$

Defining the matrices $\mathsf{U} = [\partial u^i/\partial u'^j]$, $\mathsf{G} = [g_{ij}]$ and $\mathsf{G}' = [g'_{ij}]$, we may write this expression as

$$\mathsf{G}' = \mathsf{U}^{\mathrm{T}}\mathsf{G}\mathsf{U}.$$

Taking the determinant of both sides, we obtain

$$g' = |\mathsf{U}|^2 g = \left|\frac{\partial u}{\partial u'}\right|^2 g,$$

which shows that g is a relative scalar of weight $w = 2$. ◄

From the discussion in section 26.8, it can be seen that ϵ_{ijk} is a covariant relative tensor of weight -1. We may also define the contravariant tensor ϵ^{ijk}, which is numerically equal to ϵ_{ijk} but is a relative tensor of weight $+1$.

If two relative tensors have weights w_1 and w_2 respectively then, from (26.74),

the outer product of the two tensors, or any contraction of them, is a relative tensor of weight $w_1 + w_2$. As a special case, we may use ϵ_{ijk} and ϵ^{ijk} to construct pseudovectors from antisymmetric tensors and vice versa, in an analogous way to that discussed in section 26.11.

For example, if the A^{ij} are the contravariant components of an antisymmetric tensor ($w = 0$) then

$$p_i = \tfrac{1}{2}\epsilon_{ijk}A^{jk}$$

are the covariant components of a pseudovector ($w = -1$), since ϵ_{ijk} has weight $w = -1$. Similarly, we may show that

$$A^{ij} = \epsilon^{ijk}p_k.$$

26.18 Derivatives of basis vectors and Christoffel symbols

In Cartesian coordinates, the basis vectors $\mathbf{e}_i$ are constant and so their derivatives with respect to the coordinates vanish. In a general coordinate system, however, the basis vectors $\mathbf{e}_i$ and $\mathbf{e}^i$ are functions of the coordinates. Therefore, in order that we may differentiate general tensors we must consider the derivatives of the basis vectors.

First consider the derivative $\partial\mathbf{e}_i/\partial u^j$. Since this is itself a vector, it can be written as a linear combination of the basis vectors $\mathbf{e}_k$, $k = 1, 2, 3$. If we introduce the symbol $\Gamma^k{}_{ij}$ to denote the coefficients in this combination, we have

$$\frac{\partial\mathbf{e}_i}{\partial u^j} = \Gamma^k{}_{ij}\mathbf{e}_k. \tag{26.75}$$

The coefficient $\Gamma^k{}_{ij}$ is the kth component of the vector $\partial\mathbf{e}_i/\partial u^j$. Using the reciprocity relation $\mathbf{e}^i \cdot \mathbf{e}_j = \delta^i_j$, these 27 numbers are given (at each point in space) by

$$\Gamma^k{}_{ij} = \mathbf{e}^k \cdot \frac{\partial\mathbf{e}_i}{\partial u^j}. \tag{26.76}$$

Furthermore, by differentiating the reciprocity relation $\mathbf{e}^i \cdot \mathbf{e}_j = \delta^i_j$ with respect to the coordinates, and using (26.76), it is straightforward to show that the derivatives of the contravariant basis vectors are given by

$$\frac{\partial\mathbf{e}^i}{\partial u^j} = -\Gamma^i{}_{kj}\mathbf{e}^k. \tag{26.77}$$

The symbol $\Gamma^k{}_{ij}$ is called a *Christoffel symbol* (of the second kind), but, despite appearances to the contrary, these quantities do *not* form the components of a third-order tensor. It is clear from (26.76) that in Cartesian coordinates $\Gamma^k{}_{ij} = 0$ for all values of the indices i, j and k.

►*Using (26.76), deduce the way in which the quantities* $\Gamma^k_{\ ij}$ *transform under a general coordinate transformation, and hence show that they do not form the components of a third-order tensor.*

In a new coordinate system

$$\Gamma'^k_{\ ij} = \mathbf{e}'^k \cdot \frac{\partial \mathbf{e}'_i}{\partial u'^j},$$

but from (26.69) and (26.67) respectively we have, on reversing primed and unprimed variables,

$$\mathbf{e}'^k = \frac{\partial u'^k}{\partial u^n}\mathbf{e}^n \qquad \text{and} \qquad \mathbf{e}'_i = \frac{\partial u^l}{\partial u'^i}\mathbf{e}_l.$$

Therefore in the new coordinate system the quantities $\Gamma'^k_{\ ij}$ are given by

$$\begin{aligned}
\Gamma'^k_{\ ij} &= \frac{\partial u'^k}{\partial u^n}\mathbf{e}^n \cdot \frac{\partial}{\partial u'^j}\left(\frac{\partial u^l}{\partial u'^i}\mathbf{e}_l\right) \\
&= \frac{\partial u'^k}{\partial u^n}\mathbf{e}^n \cdot \left(\frac{\partial^2 u^l}{\partial u'^j \partial u'^i}\mathbf{e}_l + \frac{\partial u^l}{\partial u'^i}\frac{\partial \mathbf{e}_l}{\partial u'^j}\right) \\
&= \frac{\partial u'^k}{\partial u^n}\frac{\partial^2 u^l}{\partial u'^j \partial u'^i}\,\mathbf{e}^n \cdot \mathbf{e}_l + \frac{\partial u'^k}{\partial u^n}\frac{\partial u^l}{\partial u'^i}\frac{\partial u^m}{\partial u'^j}\,\mathbf{e}^n \cdot \frac{\partial \mathbf{e}_l}{\partial u^m} \\
&= \frac{\partial u'^k}{\partial u^l}\frac{\partial^2 u^l}{\partial u'^j \partial u'^i} + \frac{\partial u'^k}{\partial u^n}\frac{\partial u^l}{\partial u'^i}\frac{\partial u^m}{\partial u'^j}\Gamma^n_{\ lm},
\end{aligned} \tag{26.78}$$

where in the last line we have used (26.76) and the reciprocity relation $\mathbf{e}^n \cdot \mathbf{e}_l = \delta^n_l$. From (26.78), because of the presence of the first term on the right-hand side, we conclude immediately that the $\Gamma^k_{\ ij}$ do not form the components of a third-order tensor. ◄

In a given coordinate system, in principle we may calculate the $\Gamma^k_{\ ij}$ using (26.76). In practice, however, it is often quicker to use an alternative expression, which we now derive, for the Christoffel symbol in terms of the metric tensor g_{ij} and its derivatives with respect to the coordinates.

Firstly we note that the Christoffel symbol $\Gamma^k_{\ ij}$ is symmetric with respect to the interchange of its two subscripts i and j. This is easily shown: since

$$\frac{\partial \mathbf{e}_i}{\partial u^j} = \frac{\partial^2 \mathbf{r}}{\partial u^j \partial u^i} = \frac{\partial^2 \mathbf{r}}{\partial u^i \partial u^j} = \frac{\partial \mathbf{e}_j}{\partial u^i},$$

it follows from (26.75) that $\Gamma^k_{\ ij}\mathbf{e}_k = \Gamma^k_{\ ji}\mathbf{e}_k$. Taking the scalar product with $\mathbf{e}^l$ and using the reciprocity relation $\mathbf{e}_k \cdot \mathbf{e}^l = \delta^l_k$ gives immediately that

$$\Gamma^l_{\ ij} = \Gamma^l_{\ ji}.$$

To obtain an expression for $\Gamma^k_{\ ij}$ we then use $g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$ and consider the derivative

$$\begin{aligned}
\frac{\partial g_{ij}}{\partial u^k} &= \frac{\partial \mathbf{e}_i}{\partial u^k} \cdot \mathbf{e}_j + \mathbf{e}_i \cdot \frac{\partial \mathbf{e}_j}{\partial u^k} \\
&= \Gamma^l_{\ ik}\mathbf{e}_l \cdot \mathbf{e}_j + \mathbf{e}_i \cdot \Gamma^l_{\ jk}\mathbf{e}_l \\
&= \Gamma^l_{\ ik}g_{lj} + \Gamma^l_{\ jk}g_{il},
\end{aligned} \tag{26.79}$$

where we have used the definition (26.75). By cyclically permuting the free indices i, j, k in (26.79), we obtain two further equivalent relations,

$$\frac{\partial g_{jk}}{\partial u^i} = \Gamma^l{}_{ji} g_{lk} + \Gamma^l{}_{ki} g_{jl} \tag{26.80}$$

and

$$\frac{\partial g_{ki}}{\partial u^j} = \Gamma^l{}_{kj} g_{li} + \Gamma^l{}_{ij} g_{kl}. \tag{26.81}$$

If we now add (26.80) and (26.81) together and subtract (26.79) from the result, we find

$$\begin{aligned}\frac{\partial g_{jk}}{\partial u^i} + \frac{\partial g_{ki}}{\partial u^j} - \frac{\partial g_{ij}}{\partial u^k} &= \Gamma^l{}_{ji} g_{lk} + \Gamma^l{}_{ki} g_{jl} + \Gamma^l{}_{kj} g_{li} + \Gamma^l{}_{ij} g_{kl} - \Gamma^l{}_{ik} g_{lj} - \Gamma^l{}_{jk} g_{il} \\ &= 2\Gamma^l{}_{ij} g_{kl},\end{aligned}$$

where we have used the symmetry properties of both $\Gamma^l{}_{ij}$ and g_{ij}. Contracting both sides with g^{mk} leads to the required expression for the Christoffel symbol in terms of the metric tensor and its derivatives, namely

$$\Gamma^m{}_{ij} = \tfrac{1}{2} g^{mk} \left(\frac{\partial g_{jk}}{\partial u^i} + \frac{\partial g_{ki}}{\partial u^j} - \frac{\partial g_{ij}}{\partial u^k} \right). \tag{26.82}$$

►*Calculate the Christoffel symbols $\Gamma^m{}_{ij}$ for cylindrical polar coordinates.*

We may use either (26.75) or (26.82) to calculate the $\Gamma^m{}_{ij}$ for this simple coordinate system. In cylindrical polar coordinates $(u^1, u^2, u^3) = (\rho, \phi, z)$, the basis vectors $\mathbf{e}_i$ are given by (26.59). It is straightforward to show that the only derivatives of these vectors with respect to the coordinates that are non-zero are

$$\frac{\partial \mathbf{e}_\rho}{\partial \phi} = \frac{1}{\rho}\mathbf{e}_\phi, \qquad \frac{\partial \mathbf{e}_\phi}{\partial \rho} = \frac{1}{\rho}\mathbf{e}_\phi, \qquad \frac{\partial \mathbf{e}_\phi}{\partial \phi} = -\rho \mathbf{e}_\rho.$$

Thus, from (26.75), we have immediately that

$$\Gamma^2{}_{12} = \Gamma^2{}_{21} = \frac{1}{\rho} \qquad \text{and} \qquad \Gamma^1{}_{22} = -\rho. \tag{26.83}$$

Alternatively, using (26.82) and the fact that $g_{11} = 1$, $g_{22} = \rho^2$, $g_{33} = 1$ and the other components are zero, we see that the only three non-zero Christoffel symbols are indeed $\Gamma^2{}_{12} = \Gamma^2{}_{21}$ and $\Gamma^1{}_{22}$. These are given by

$$\Gamma^2{}_{12} = \Gamma^2{}_{21} = \frac{1}{2g_{22}} \frac{\partial g_{22}}{\partial u^1} = \frac{1}{2\rho^2} \frac{\partial}{\partial \rho}(\rho^2) = \frac{1}{\rho},$$

$$\Gamma^1{}_{22} = -\frac{1}{2g_{11}} \frac{\partial g_{22}}{\partial u^1} = -\frac{1}{2} \frac{\partial}{\partial \rho}(\rho^2) = -\rho,$$

which agree with the expressions found directly from (26.75) and given in (26.83). ◄

26.19 Covariant differentiation

For Cartesian tensors we noted that the derivative of a scalar is a (covariant) vector. This is also true for *general* tensors, as may be shown by considering the differential of a scalar

$$d\phi = \frac{\partial \phi}{\partial u^i}\, du^i.$$

Since the du^i are the components of a contravariant vector and $d\phi$ is a scalar, we have by the quotient law, discussed in section 26.7, that the quantities $\partial\phi/\partial u^i$ must form the components of a covariant vector. As a second example, if the contravariant components in Cartesian coordinates of a vector $\mathbf{v}$ are v^i, then the quantities $\partial v^i/\partial x^j$ form the components of a second-order tensor.

However, it is straightforward to show that in non-Cartesian coordinates differentiation of the components of a general tensor, other than a scalar, with respect to the coordinates does *not* in general result in the components of another tensor.

►*Show that, in* general *coordinates, the quantities* $\partial v^i/\partial u^j$ *do not form the components of a tensor.*

We may show this directly by considering

$$\begin{aligned}\left(\frac{\partial v^i}{\partial u^j}\right)' = \frac{\partial v'^i}{\partial u'^j} &= \frac{\partial u^k}{\partial u'^j}\frac{\partial v'^i}{\partial u^k} \\ &= \frac{\partial u^k}{\partial u'^j}\frac{\partial}{\partial u^k}\left(\frac{\partial u'^i}{\partial u^l}v^l\right) \\ &= \frac{\partial u^k}{\partial u'^j}\frac{\partial u'^i}{\partial u^l}\frac{\partial v^l}{\partial u^k} + \frac{\partial u^k}{\partial u'^j}\frac{\partial^2 u'^i}{\partial u^k \partial u^l}v^l. \end{aligned} \tag{26.84}$$

The presence of the second term on the right-hand side of (26.84) shows that the $\partial v^i/\partial x^j$ do not form the components of a second-order tensor. This term arises because the 'transformation matrix' $[\partial u'^i/\partial u^j]$ changes as the position in space at which it is evaluated is changed. This is not true in Cartesian coordinates, for which the second term vanishes and $\partial v^i/\partial x^j$ is a second-order tensor. ◄

We may, however, use the Christoffel symbols discussed in the previous section to define a new *covariant* derivative of the components of a tensor that does result in the components of another tensor.

Let us first consider the derivative of a vector $\mathbf{v}$ with respect to the coordinates. Writing the vector in terms of its contravariant components $\mathbf{v} = v^i\mathbf{e}_i$, we find

$$\frac{\partial \mathbf{v}}{\partial u^j} = \frac{\partial v^i}{\partial u^j}\mathbf{e}_i + v^i\frac{\partial \mathbf{e}_i}{\partial u^j}, \tag{26.85}$$

where the second term arises because, in general, the basis vectors $\mathbf{e}_i$ are not

constant (this term vanishes in Cartesian coordinates). Using (26.75) we write

$$\frac{\partial \mathbf{v}}{\partial u^j} = \frac{\partial v^i}{\partial u^j}\mathbf{e}_i + v^i \Gamma^k{}_{ij}\mathbf{e}_k.$$

Since i and k are dummy indices in the last term on the right-hand side, we may interchange them to obtain

$$\frac{\partial \mathbf{v}}{\partial u^j} = \frac{\partial v^i}{\partial u^j}\mathbf{e}_i + v^k \Gamma^i{}_{kj}\mathbf{e}_i = \left(\frac{\partial v^i}{\partial u^j} + v^k \Gamma^i{}_{kj}\right)\mathbf{e}_i. \tag{26.86}$$

The reason for the interchanging the dummy indices, as shown in (26.86), is that we may now factor out $\mathbf{e}_i$. The quantity in parentheses is called the *covariant derivative*, for which the standard notation is

$$v^i{}_{;j} \equiv \frac{\partial v^i}{\partial u^j} + \Gamma^i{}_{kj} v^k, \tag{26.87}$$

the semicolon subscript denoting covariant differentiation. A similar short-hand notation also exists for the partial derivatives, a comma being used for these instead of a semicolon; for example, $\partial v^i/\partial u^j$ is denoted by $v^i{}_{,j}$. In Cartesian coordinates all the $\Gamma^i{}_{kj}$ are zero, and so the covariant derivative reduces to the simple partial derivative $\partial v^i/\partial u^j$.

Using the short-hand semicolon notation, the derivative of a vector may be written in the very compact form

$$\frac{\partial \mathbf{v}}{\partial u^j} = v^i{}_{;j}\mathbf{e}_i$$

and, by the quotient rule (section 26.7), it is clear that the $v^i{}_{;j}$ are the (mixed) components of a second-order tensor. This may also be verified directly, using the transformation properties of $\partial v^i/\partial u^j$ and $\Gamma^i{}_{kj}$ given in (26.84) and (26.78) respectively.

In general, we may regard the $v^i{}_{;j}$ as the mixed components of a second-order tensor called the covariant derivative of $\mathbf{v}$ and denoted by $\nabla\mathbf{v}$. In Cartesian coordinates, the components of this tensor are just $\partial v^i/\partial x^j$.

►*Calculate $v^i{}_{;i}$ in cylindrical polar coordinates.*

Contracting (26.87) we obtain

$$v^i{}_{;i} = \frac{\partial v^i}{\partial u^i} + \Gamma^i{}_{ki} v^k.$$

Now from (26.83) we have

$$\begin{aligned}
\Gamma^i{}_{1i} &= \Gamma^1{}_{11} + \Gamma^2{}_{12} + \Gamma^3{}_{13} = 1/\rho, \\
\Gamma^i{}_{2i} &= \Gamma^1{}_{21} + \Gamma^2{}_{22} + \Gamma^3{}_{23} = 0, \\
\Gamma^i{}_{3i} &= \Gamma^1{}_{31} + \Gamma^2{}_{32} + \Gamma^3{}_{33} = 0,
\end{aligned}$$

and so

$$v^i{}_{;i} = \frac{\partial v^\rho}{\partial \rho} + \frac{\partial v^\phi}{\partial \phi} + \frac{\partial v^z}{\partial z} + \frac{1}{\rho} v^\rho$$
$$= \frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho v^\rho) + \frac{\partial v^\phi}{\partial \phi} + \frac{\partial v^z}{\partial z}.$$

This result is identical to the expression for the divergence of a vector field in cylindrical polar coordinates given in section 10.9. This is discussed further in section 26.20. ◄

So far we have considered only the covariant derivative of the contravariant components v^i of a vector. The corresponding result for the covariant components v_i may be found in a similar way, by considering the derivative of $\mathbf{v} = v_i \mathbf{e}^i$ and using (26.77) to obtain

$$v_{i;j} = \frac{\partial v_i}{\partial u^j} - \Gamma^k{}_{ij} v_k. \tag{26.88}$$

Comparing the expressions (26.87) and (26.88) for the covariant derivative of the contravariant and covariant components of a vector respectively, we see that there are some similarities and some differences. It may help to remember that the index with respect to which the covariant derivative is taken (j in this case), is also the last subscript on the Christoffel symbol; the remaining indices can then be arranged in only one way without raising or lowering them. It only remains to note that for a covariant index (subscript) the Christoffel symbol carries a minus sign, whereas for a contravariant index (superscript) the sign is positive.

Following a similar procedure to that which led to equation (26.87), we may obtain expressions for the covariant derivatives of higher-order tensors.

► *By considering the derivative of the second-order tensor* $\mathbf{T}$ *with respect to the coordinate* u^k*, find an expression for the covariant derivative* $T^{ij}{}_{;k}$ *of its contravariant components.*

Expressing $\mathbf{T}$ in terms of its contravariant components, we have

$$\frac{\partial \mathbf{T}}{\partial u^k} = \frac{\partial}{\partial u^k}(T^{ij}\mathbf{e}_i \otimes \mathbf{e}_j)$$
$$= \frac{\partial T^{ij}}{\partial u^k}\mathbf{e}_i \otimes \mathbf{e}_j + T^{ij}\frac{\partial \mathbf{e}_i}{\partial u^k} \otimes \mathbf{e}_j + T^{ij}\mathbf{e}_i \otimes \frac{\partial \mathbf{e}_j}{\partial u^k}.$$

Using (26.75), we can rewrite the derivatives of the basis vectors in terms of Christoffel symbols to obtain

$$\frac{\partial \mathbf{T}}{\partial u^k} = \frac{\partial T^{ij}}{\partial u^k}\mathbf{e}_i \otimes \mathbf{e}_j + T^{ij}\Gamma^l{}_{ik}\mathbf{e}_l \otimes \mathbf{e}_j + T^{ij}\mathbf{e}_i \otimes \Gamma^l{}_{jk}\mathbf{e}_l.$$

Interchanging the dummy indices i and l in the second term and j and l in the third term on the right-hand side, this becomes

$$\frac{\partial \mathbf{T}}{\partial u^k} = \left(\frac{\partial T^{ij}}{\partial u^k} + \Gamma^i{}_{lk}T^{lj} + \Gamma^j{}_{lk}T^{il}\right)\mathbf{e}_i \otimes \mathbf{e}_j,$$

where the expression in parentheses is the required covariant derivative

$$T^{ij}{}_{;k} = \frac{\partial T^{ij}}{\partial u^k} + \Gamma^i{}_{lk}T^{lj} + \Gamma^j{}_{lk}T^{il}. \tag{26.89}$$

Using (26.89), the derivative of the tensor $\mathbf{T}$ with respect to u^k can now be written in terms of its contravariant components as

$$\frac{\partial \mathbf{T}}{\partial u^k} = T^{ij}{}_{;k}\mathbf{e}_i \otimes \mathbf{e}_j. \blacktriangleleft$$

Results similar to (26.89) may be obtained for the the covariant derivatives of the mixed and covariant components of a second-order tensor. Collecting these results together, we have

$$\begin{aligned} T^{ij}{}_{;k} &= T^{ij}{}_{,k} + \Gamma^i{}_{lk}T^{lj} + \Gamma^j{}_{lk}T^{il}, \\ T^i{}_{j;k} &= T^i{}_{j,k} + \Gamma^i{}_{lk}T^l{}_j - \Gamma^l{}_{jk}T^i{}_l, \\ T_{ij;k} &= T_{ij,k} - \Gamma^l{}_{ik}T_{lj} - \Gamma^l{}_{jk}T_{il}, \end{aligned}$$

where we have used the comma notation for partial derivatives. The position of the indices in these expressions is very systematic: for each contravariant index (superscript) on the LHS we add a term on the RHS containing a Christoffel symbol with a plus sign, and for every covariant index (subscript) we add a corresponding term with a minus sign. This is extended straightforwardly to tensors with an arbitrary number of contravariant and covariant indices.

We note that the quantities $T^{ij}{}_{;k}$, $T^i{}_{j;k}$ and $T_{ij;k}$ are the components of the *same* third-order tensor $\nabla\mathbf{T}$ with respect to different tensor bases, i.e.

$$\nabla\mathbf{T} = T^{ij}{}_{;k}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}^k = T^i{}_{j;k}\mathbf{e}_i \otimes \mathbf{e}^j \otimes \mathbf{e}^k = T_{ij;k}\mathbf{e}^i \otimes \mathbf{e}^j \otimes \mathbf{e}^k.$$

We conclude this section by considering briefly the covariant derivative of a scalar. The covariant derivative differs from the simple partial derivative with respect to the coordinates only because the basis vectors of the coordinate system change with position in space (hence for Cartesian coordinates there is no difference). However, a scalar ϕ does not depend on the basis vectors at all and so its covariant derivative must be the same as its partial derivative, i.e.

$$\phi_{;j} = \frac{\partial \phi}{\partial u^j} = \phi_{,j}. \tag{26.90}$$

26.20 Vector operators in tensor form

In section 10.10 we used vector calculus methods to find expressions for vector differential operators, such as grad, div, curl and the Laplacian, in general *orthogonal* curvilinear coordinates, taking cylindrical and spherical polars as particular examples. In this section we use the framework of general tensors that we have developed to obtain, in tensor form, expressions for these operators that are valid in *all* coordinate systems, whether orthogonal or not.

In order to compare the results obtained here with those given in section 10.10 for orthogonal coordinates, it is necessary to remember that here we are working with the (in general) non-unit basis vectors $\mathbf{e}_i = \partial\mathbf{r}/\partial u^i$ or $\mathbf{e}^i = \nabla u^i$. Thus the components of a vector $\mathbf{v} = v^i\mathbf{e}_i$ are not the same as the components $\hat{v}^i$ appropriate to the corresponding unit basis $\hat{\mathbf{e}}_i$. In fact, if the scale factors of the coordinate system are h_i, $i = 1, 2, 3$, then $v^i = \hat{v}^i/h_i$ (no summation over i).

As mentioned in section 26.15, for an orthogonal coordinate system with scale factors h_i we have

$$g_{ij} = \begin{cases} h_i^2 & \text{if } i = j, \\ 0 & \text{otherwise} \end{cases} \qquad \text{and} \qquad g^{ij} = \begin{cases} 1/h_i^2 & \text{if } i = j, \\ 0 & \text{otherwise,} \end{cases}$$

and so the determinant g of the matrix $[g_{ij}]$ is given by $g = h_1^2h_2^2h_3^2$.

Gradient

The gradient of a scalar ϕ is given by

$$\nabla\phi = \phi_{;i}\mathbf{e}^i = \frac{\partial\phi}{\partial u^i}\mathbf{e}^i, \tag{26.91}$$

since the covariant derivative of a scalar is the same as its partial derivative.

Divergence

Replacing the partial derivatives that occur in Cartesian coordinates with covariant derivatives, the divergence of a vector field $\mathbf{v}$ in a general coordinate system is given by

$$\nabla\cdot\mathbf{v} = v^i{}_{;i} = \frac{\partial v^i}{\partial u^i} + \Gamma^i_{ki}v^k.$$

Using the expression (26.82) for the Christoffel symbol in terms of the metric tensor, we find

$$\Gamma^i_{ki} = \tfrac{1}{2}g^{il}\left(\frac{\partial g_{il}}{\partial u^k} + \frac{\partial g_{kl}}{\partial u^i} - \frac{\partial g_{ki}}{\partial u^l}\right) = \tfrac{1}{2}g^{il}\frac{\partial g_{il}}{\partial u^k}. \tag{26.92}$$

The last two terms have cancelled because

$$g^{il}\frac{\partial g_{kl}}{\partial u^i} = g^{li}\frac{\partial g_{ki}}{\partial u^l} = g^{il}\frac{\partial g_{ki}}{\partial u^l},$$

where in the first equality we have interchanged the dummy indices i and l, and in the second equality have used the symmetry of the metric tensor.

We may simplify (26.92) still further by using a result concerning the derivative of the determinant of a matrix whose elements are functions of the coordinates.

►*Suppose* $\mathsf{A} = [a_{ij}]$, $\mathsf{B} = [b^{ij}]$ *and that* $\mathsf{B} = \mathsf{A}^{-1}$. *By considering the determinant* $a = |\mathsf{A}|$, *show that*

$$\frac{\partial a}{\partial u^k} = ab^{ji}\frac{\partial a_{ij}}{\partial u^k}.$$

If we denote the cofactor of the element a_{ij} by Δ^{ij} then the elements of the inverse matrix are given by (see chapter 8)

$$b^{ij} = \frac{1}{a}\Delta^{ji}. \tag{26.93}$$

However, the determinant of A is given by

$$a = \sum_j a_{ij}\Delta^{ij},$$

in which we have *fixed* i and written the sum over j explicitly, for clarity. Partially differentiating both sides with respect to a_{ij}, we then obtain

$$\frac{\partial a}{\partial a_{ij}} = \Delta^{ij}, \tag{26.94}$$

since a_{ij} does not occur in any of the cofactors Δ^{ij}.

Now, if the a_{ij} depend on the coordinates then so will the determinant a and, by the chain rule, we have

$$\frac{\partial a}{\partial u^k} = \frac{\partial a}{\partial a_{ij}}\frac{\partial a_{ij}}{\partial u^k} = \Delta^{ij}\frac{\partial a_{ij}}{\partial u^k} = ab^{ji}\frac{\partial a_{ij}}{\partial u^k}, \tag{26.95}$$

in which we have used (26.93) and (26.94). ◄

Applying the result (26.95) to the determinant g of the metric tensor, and remembering both that $g^{ik}g_{kj} = \delta^i_j$ and that g^{ij} is symmetric, we obtain

$$\frac{\partial g}{\partial u^k} = gg^{ij}\frac{\partial g_{ij}}{\partial u^k}. \tag{26.96}$$

Substituting (26.96) into (26.92) we find that the expression for the Christoffel symbol can be much simplified to give

$$\Gamma^i_{\ ki} = \frac{1}{2g}\frac{\partial g}{\partial u^k} = \frac{1}{\sqrt{g}}\frac{\partial\sqrt{g}}{\partial u^k}.$$

Thus finally we obtain the expression for the divergence of a vector field in a general coordinate system as

$$\nabla\cdot\mathbf{v} = v^i{}_{;i} = \frac{1}{\sqrt{g}}\frac{\partial}{\partial u^j}(\sqrt{g}v^j). \tag{26.97}$$

Laplacian

If we replace $\mathbf{v}$ by $\nabla\phi$ in $\nabla\cdot\mathbf{v}$ then we obtain the Laplacian $\nabla^2\phi$. From (26.91), we have

$$v_i\mathbf{e}^i = \mathbf{v} = \nabla\phi = \frac{\partial\phi}{\partial u^i}\mathbf{e}^i,$$

and so the covariant components of $\mathbf{v}$ are given by $v_i = \partial\phi/\partial u^i$. In (26.97), however, we require the contravariant components v^i. These may be obtained by raising the index using the metric tensor, to give

$$v^j = g^{jk} v_k = g^{jk} \frac{\partial \phi}{\partial u^k}.$$

Substituting this into (26.97) we obtain

$$\nabla^2 \phi = \frac{1}{\sqrt{g}} \frac{\partial}{\partial u^j} \left(\sqrt{g} g^{jk} \frac{\partial \phi}{\partial u^k} \right). \tag{26.98}$$

►*Use (26.98) to find the expression for $\nabla^2\phi$ in an orthogonal coordinate system with scale factors h_i, $i = 1, 2, 3$.*

For an orthogonal coordinate system $\sqrt{g} = h_1 h_2 h_3$; further, $g^{ij} = 1/h_i^2$ if $i = j$ and $g^{ij} = 0$ otherwise. Therefore, from (26.98) we have

$$\nabla^2 \phi = \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial u^j} \left(\frac{h_1 h_2 h_3}{h_j^2} \frac{\partial \phi}{\partial u^j} \right),$$

which agrees with the results of section 10.10. ◄

Curl

The special vector form of the curl of a vector field exists only in three dimensions. We therefore consider a more general form valid in higher-dimensional spaces as well. In a general space the operation curl $\mathbf{v}$ is defined by

$$(\text{curl } \mathbf{v})_{ij} = v_{i;j} - v_{j;i},$$

which is an antisymmetric covariant tensor.

In fact the difference of derivatives can be simplified, since

$$\begin{aligned} v_{i;j} - v_{j;i} &= \frac{\partial v_i}{\partial u^j} - \Gamma^l{}_{ij} v_l - \frac{\partial v_j}{\partial u^i} + \Gamma^l{}_{ji} v_l \\ &= \frac{\partial v_i}{\partial u^j} - \frac{\partial v_j}{\partial u^i}, \end{aligned}$$

where the Christoffel symbols have cancelled because of their symmetry properties. Thus curl $\mathbf{v}$ can be written in terms of partial derivatives as

$$(\text{curl } \mathbf{v})_{ij} = \frac{\partial v_i}{\partial u^j} - \frac{\partial v_j}{\partial u^i}.$$

Generalising slightly the discussion of section 26.17, in three dimensions we may associate with this antisymmetric second-order tensor a vector with contravariant components,

$$\begin{aligned} (\nabla \times \mathbf{v})^i &= -\frac{1}{2\sqrt{g}} \epsilon^{ijk} (\text{curl } \mathbf{v})_{jk} \\ &= -\frac{1}{2\sqrt{g}} \epsilon^{ijk} \left(\frac{\partial v_j}{\partial u^k} - \frac{\partial v_k}{\partial u^j} \right) = \frac{1}{\sqrt{g}} \epsilon^{ijk} \frac{\partial v_k}{\partial u^j}; \end{aligned}$$

this is the analogue of the expression in Cartesian coordinates discussed in section 26.8.

26.21 Absolute derivatives along curves

In section 26.19 we discussed how to differentiate a general tensor with respect to the coordinates and introduced the covariant derivative. In this section we consider the slightly different problem of calculating the derivative of a tensor along a curve $\mathbf{r}(t)$ that is parameterised by some variable t.

Let us begin by considering the derivative of a vector $\mathbf{v}$ along the curve. If we introduce an arbitrary coordinate system u^i with basis vectors $\mathbf{e}_i$, $i = 1, 2, 3$, then we may write $\mathbf{v} = v^i\mathbf{e}_i$ and so obtain

$$\begin{aligned}\frac{d\mathbf{v}}{dt} &= \frac{dv^i}{dt}\mathbf{e}_i + v^i\frac{d\mathbf{e}_i}{dt} \\ &= \frac{dv^i}{dt}\mathbf{e}_i + v^i\frac{\partial\mathbf{e}_i}{\partial u^k}\frac{du^k}{dt};\end{aligned}$$

here the chain rule has been used to rewrite the last term on the right-hand side. Using (26.75) to write the derivatives of the basis vectors in terms of Christoffel symbols, we obtain

$$\frac{d\mathbf{v}}{dt} = \frac{dv^i}{dt}\mathbf{e}_i + \Gamma^j{}_{ik}v^i\frac{du^k}{dt}\mathbf{e}_j.$$

Interchanging the dummy indices i and j in the last term, we may factor out the basis vector and find

$$\frac{d\mathbf{v}}{dt} = \left(\frac{dv^i}{dt} + \Gamma^i{}_{jk}v^j\frac{du^k}{dt}\right)\mathbf{e}_i.$$

The term in parentheses is called the *absolute* (or *intrinsic*) derivative of the components v^i along the curve $\mathbf{r}(t)$and is usually denoted by

$$\frac{\delta v^i}{\delta t} \equiv \frac{dv^i}{dt} + \Gamma^i{}_{jk}v^j\frac{du^k}{dt} = v^i{}_{;k}\frac{du^k}{dt}.$$

With this notation, we may write

$$\frac{d\mathbf{v}}{dt} = \frac{\delta v^i}{\delta t}\mathbf{e}_i = v^i{}_{;k}\frac{du^k}{dt}\mathbf{e}_i. \tag{26.99}$$

Using the same method, the absolute derivative of the covariant components v_i of a vector is given by

$$\frac{\delta v_i}{\delta t} \equiv v_{i;k}\frac{du^k}{dt}.$$

Similarly, the absolute derivatives of the contravariant, mixed and covariant

components of a second-order tensor $\mathbf{T}$ are

$$\frac{\delta T^{ij}}{\delta t} \equiv T^{ij}{}_{;k}\frac{du^k}{dt},$$
$$\frac{\delta T^{i}{}_{j}}{\delta t} \equiv T^{i}{}_{j;k}\frac{du^k}{dt},$$
$$\frac{\delta T_{ij}}{\delta t} \equiv T_{ij;k}\frac{du^k}{dt}.$$

The derivative of $\mathbf{T}$ along the curve $\mathbf{r}(t)$ may then be written in terms of, for example, its contravariant components as

$$\frac{d\mathbf{T}}{dt} = \frac{\delta T^{ij}}{\delta t}\mathbf{e}_i \otimes \mathbf{e}_j = T^{ij}{}_{;k}\frac{du^k}{dt}\mathbf{e}_i \otimes \mathbf{e}_j.$$

26.22 Geodesics

As an example of the use of the absolute derivative, we conclude this chapter with a brief discussion of geodesics. A geodesic in real three-dimensional space is a straight line, which has two equivalent defining properties. Firstly, it is the curve of shortest length between two points and, secondly, it is the curve whose tangent vector always points in the same direction (along the line). Although in this chapter we have considered explicitly only our familiar three-dimensional space, much of the mathematical formalism developed can be generalised to more abstract spaces of higher dimensionality in which the familiar ideas of Euclidean geometry are no longer valid. It is often of interest to find geodesic curves in such spaces by using the defining properties of straight lines in Euclidean space.

We shall not consider these more complicated spaces explicitly but will determine the equation that a geodesic in Euclidean three-dimensional space (i.e. a straight line) must satisfy, deriving it in a sufficiently general way that our method may be applied with little modification to finding the equations satisfied by geodesics in more abstract spaces.

Let us consider a curve $\mathbf{r}(s)$, parameterised by the arc length s from some point on the curve, and choose as our defining property for a geodesic that its tangent vector $\mathbf{t} = d\mathbf{r}/ds$ always points in the same direction everywhere on the curve, i.e.

$$\frac{d\mathbf{t}}{ds} = \mathbf{0}. \tag{26.100}$$

Alternatively, we could exploit the property that the distance between two points is a minimum along a geodesic and use the calculus of variations (see chapter 22); this would lead to the same final result (26.101).

If we now introduce an arbitrary coordinate system u^i with basis vectors $\mathbf{e}_i$, $i = 1, 2, 3$, then we may write $\mathbf{t} = t^i\mathbf{e}_i$, and from (26.99) we find

$$\frac{d\mathbf{t}}{ds} = t^i{}_{;k}\frac{du^k}{ds}\mathbf{e}_i = \mathbf{0}.$$

Writing out the covariant derivative, we obtain

$$\left(\frac{dt^i}{ds} + \Gamma^i{}_{jk} t^j \frac{du^k}{ds}\right) \mathbf{e}_i = \mathbf{0}.$$

But, since $t^j = du^j/ds$, it follows that the equation satisfied by a geodesic is

$$\frac{d^2u^i}{ds^2} + \Gamma^i{}_{jk} \frac{du^j}{ds}\frac{du^k}{ds} = 0. \tag{26.101}$$

►*Find the equations satisfied by a geodesic (straight line) in cylindrical polar coordinates.*

From (26.83), the only non-zero Christoffel symbols are $\Gamma^1{}_{22} = -\rho$ and $\Gamma^2{}_{12} = \Gamma^2{}_{21} = 1/\rho$. Thus the required geodesic equations are

$$\begin{aligned}
\frac{d^2u^1}{ds^2} + \Gamma^1{}_{22}\frac{du^2}{ds}\frac{du^2}{ds} = 0 \quad &\Rightarrow \quad \frac{d^2\rho}{ds^2} - \rho\left(\frac{d\phi}{ds}\right)^2 = 0, \\
\frac{d^2u^2}{ds^2} + 2\Gamma^2{}_{12}\frac{du^1}{ds}\frac{du^2}{ds} = 0 \quad &\Rightarrow \quad \frac{d^2\phi}{ds^2} + \frac{2}{\rho}\frac{d\rho}{ds}\frac{d\phi}{ds} = 0, \\
\frac{d^2u^3}{ds^2} = 0 \quad &\Rightarrow \quad \frac{d^2z}{ds^2} = 0. \ \blacktriangleleft
\end{aligned}$$

26.23 Exercises

26.1 Use the basic definition of a Cartesian tensor to show the following.

(a) That for any general, but fixed, ϕ,

$$(u_1, u_2) = (x_1\cos\phi - x_2\sin\phi,\ x_1\sin\phi + x_2\cos\phi)$$

are the components of a first-order tensor in two dimensions.

(b) That

$$\begin{pmatrix} x_2^2 & x_1x_2 \\ x_1x_2 & x_1^2 \end{pmatrix}$$

is not a tensor of order 2. To establish that a single element does not transform correctly is sufficient.

26.2 The components of two vectors, **A** and **B**, and a second-order tensor, **T**, are given in one coordinate system by

$$\mathsf{A} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathsf{B} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathsf{T} = \begin{pmatrix} 2 & \sqrt{3} & 0 \\ \sqrt{3} & 4 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

In a second coordinate system, obtained from the first by rotation, the components of **A** and **B** are

$$\mathsf{A}' = \frac{1}{2}\begin{pmatrix} \sqrt{3} \\ 0 \\ 1 \end{pmatrix}, \quad \mathsf{B}' = \frac{1}{2}\begin{pmatrix} -1 \\ 0 \\ \sqrt{3} \end{pmatrix}.$$

Find the components of **T** in this new coordinate system and hence evaluate, with a minimum of calculation,

$$T_{ij}T_{ji}, \quad T_{ki}T_{jk}T_{ij}, \quad T_{ik}T_{mn}T_{ni}T_{km}.$$

26.3 In section 26.3 the transformation matrix for a rotation of the coordinate axes was derived, and this approach is used in the rest of the chapter. An alternative view is that of taking the coordinate axes as fixed and rotating the components of the system; this is equivalent to reversing the signs of all rotation angles.

Using this alternative view, determine the matrices representing (a) a positive rotation of $\pi/4$ about the x-axis and (b) a rotation of $-\pi/4$ about the y-axis. Determine the initial vector $\mathbf{r}$ which, when subjected to (a) followed by (b), finishes at $(3, 2, 1)$.

26.4 Show how to decompose the Cartesian tensor T_{ij} into three tensors,

$$T_{ij} = U_{ij} + V_{ij} + S_{ij},$$

where U_{ij} is symmetric and has zero trace, V_{ij} is isotropic and S_{ij} has only three independent components.

26.5 Use the quotient law discussed in section 26.7 to show that the array

$$\begin{pmatrix} y^2+z^2-x^2 & -2xy & -2xz \\ -2yx & x^2+z^2-y^2 & -2yz \\ -2zx & -2zy & x^2+y^2-z^2 \end{pmatrix}$$

forms a second-order tensor.

26.6 Use tensor methods to establish the following vector identities:

(a) $(\mathbf{u}\times\mathbf{v})\times\mathbf{w} = (\mathbf{u}\cdot\mathbf{w})\mathbf{v} - (\mathbf{v}\cdot\mathbf{w})\mathbf{u}$;
(b) $\operatorname{curl}(\phi\mathbf{u}) = \phi\operatorname{curl}\mathbf{u} + (\operatorname{grad}\phi)\times\mathbf{u}$;
(c) $\operatorname{div}(\mathbf{u}\times\mathbf{v}) = \mathbf{v}\cdot\operatorname{curl}\mathbf{u} - \mathbf{u}\cdot\operatorname{curl}\mathbf{v}$;
(d) $\operatorname{curl}(\mathbf{u}\times\mathbf{v}) = (\mathbf{v}\cdot\operatorname{grad})\mathbf{u} - (\mathbf{u}\cdot\operatorname{grad})\mathbf{v} + \mathbf{u}\operatorname{div}\mathbf{v} - \mathbf{v}\operatorname{div}\mathbf{u}$;
(e) $\operatorname{grad}\frac{1}{2}(\mathbf{u}\cdot\mathbf{u}) = \mathbf{u}\times\operatorname{curl}\mathbf{u} + (\mathbf{u}\cdot\operatorname{grad})\mathbf{u}$.

26.7 Use result (e) of the previous question and the general divergence theorem for tensors to show that, for a vector field $\mathbf{A}$,

$$\int_S \left[\mathbf{A}(\mathbf{A}\cdot d\mathbf{S}) - \tfrac{1}{2}A^2 d\mathbf{S}\right] = \int_V \left[\mathbf{A}\,\mathrm{div}\mathbf{A} - \mathbf{A}\times\operatorname{curl}\mathbf{A}\right] dV,$$

where S is the surface enclosing volume V.

26.8 A column matrix a has components a_x, a_y, a_z and A is the matrix with elements $A_{ij} = -\epsilon_{ijk}a_k$.

(a) What is the relationship between column matrices b and c if $\mathsf{Ab} = \mathsf{c}$?
(b) Find the eigenvalues of A and show that a is one of its eigenvectors. Explain why this must be so.

26.9 Equation (26.29),

$$|\mathsf{A}|\epsilon_{lmn} = A_{li}A_{mj}A_{nk}\epsilon_{ijk},$$

is a more general form of the expression (8.47) for the determinant of a 3×3 matrix A. The latter could have been written as

$$|\mathsf{A}| = \epsilon_{ijk}A_{i1}A_{j2}A_{k3},$$

whilst the former removes the explicit mention of $1, 2, 3$ at the expense of an additional Levi–Civita symbol. As stated in the footnote on p. 942, (26.29) can be readily extended to cover a general $N\times N$ matrix.

Use the form given in (26.29) to prove properties (i), (iii), (v), (vi) and (vii) of determinants stated in subsection 8.9.1. Property (iv) is obvious by inspection. For definiteness take $N = 3$, but convince yourself that your methods of proof would be valid for any positive integer N.

26.10 A symmetric second-order Cartesian tensor is defined by

$$T_{ij} = \delta_{ij} - 3x_i x_j.$$

Evaluate the following surface integrals, each taken over the surface of the unit sphere:

$$\text{(a)} \int T_{ij}\, dS; \quad \text{(b)} \int T_{ik} T_{kj}\, dS; \quad \text{(c)} \int x_i T_{jk}\, dS.$$

26.11 Given a non-zero vector $\mathbf{v}$, find the value that should be assigned to α to make

$$P_{ij} = \alpha v_i v_j \qquad \text{and} \qquad Q_{ij} = \delta_{ij} - \alpha v_i v_j$$

into parallel and orthogonal projection tensors, respectively, i.e. tensors that satisfy, respectively, $P_{ij}v_j = v_i$, $P_{ij}u_j = 0$ and $Q_{ij}v_j = 0$, $Q_{ij}u_j = u_i$, for any vector $\mathbf{u}$ that is orthogonal to $\mathbf{v}$.

Show, in particular, that Q_{ij} is unique, i.e. that if another tensor T_{ij} has the same properties as Q_{ij} then $(Q_{ij} - T_{ij})w_j = 0$ for *any* vector $\mathbf{w}$.

26.12 In four dimensions, define second-order antisymmetric tensors, F_{ij} and Q_{ij}, and a first-order tensor, S_i, as follows:

(a) $F_{23} = H_1$, $Q_{23} = B_1$ and their cyclic permutations;
(b) $F_{i4} = -D_i$, $Q_{i4} = E_i$ for $i = 1, 2, 3$;
(c) $S_4 = \rho$, $S_i = J_i$ for $i = 1, 2, 3$.

Then, taking x_4 as t and the other symbols to have their usual meanings in electromagnetic theory, show that the equations $\sum_j \partial F_{ij}/\partial x_j = S_i$ and $\partial Q_{jk}/\partial x_i + \partial Q_{ki}/\partial x_j + \partial Q_{ij}/\partial x_k = 0$ reproduce Maxwell's equations. In the latter i, j, k is any set of three subscripts selected from 1, 2, 3, 4, but chosen in such a way that they are all different.

26.13 In a certain crystal the unit cell can be taken as six identical atoms lying at the corners of a regular octahedron. Convince yourself that these atoms can also be considered as lying at the centres of the faces of a cube and hence that the crystal has cubic symmetry. Use this result to *prove* that the conductivity tensor for the crystal, σ_{ij}, must be isotropic.

26.14 Assuming that the current density $\mathbf{j}$ and the electric field $\mathbf{E}$ appearing in equation (26.44) are first-order Cartesian tensors, show explicitly that the electrical conductivity tensor σ_{ij} transforms according to the law appropriate to a second-order tensor.

The rate W at which energy is dissipated per unit volume, as a result of the current flow, is given by $\mathbf{E} \cdot \mathbf{j}$. Determine the limits between which W must lie for a given value of $|\mathbf{E}|$ as the direction of $\mathbf{E}$ is varied.

26.15 In a certain system of units, the electromagnetic stress tensor M_{ij} is given by

$$M_{ij} = E_i E_j + B_i B_j - \tfrac{1}{2}\delta_{ij}(E_k E_k + B_k B_k),$$

where the electric and magnetic fields, $\mathbf{E}$ and $\mathbf{B}$, are first-order tensors. Show that M_{ij} is a second-order tensor.

Consider a situation in which $|\mathbf{E}| = |\mathbf{B}|$, but the directions of $\mathbf{E}$ and $\mathbf{B}$ are not parallel. Show that $\mathbf{E} \pm \mathbf{B}$ are principal axes of the stress tensor and find the corresponding principal values. Determine the third principal axis and its corresponding principal value.

26.16 A rigid body consists of four particles of masses m, $2m$, $3m$, $4m$, respectively situated at the points (a, a, a), $(a, -a, -a)$, $(-a, a, -a)$, $(-a, -a, a)$ and connected together by a light framework.

(a) Find the inertia tensor at the origin and show that the principal moments of inertia are $20ma^2$ and $(20 \pm 2\sqrt{5})ma^2$.

(b) Find the principal axes and verify that they are orthogonal.

26.17 A rigid body consists of eight particles, each of mass m, held together by light rods. In a certain coordinate frame the particles are at positions

$$\pm a(3,1,-1), \qquad \pm a(1,-1,3), \qquad \pm a(1,3,-1), \qquad \pm a(-1,1,3).$$

Show that, when the body rotates about an axis through the origin, if the angular velocity and angular momentum vectors are parallel then their ratio must be $40ma^2$, $64ma^2$ or $72ma^2$.

26.18 The paramagnetic tensor χ_{ij} of a body placed in a magnetic field, in which its energy density is $-\frac{1}{2}\mu_0 \mathbf{M}\cdot\mathbf{H}$ with $M_i = \sum_j \chi_{ij} H_j$, is

$$\begin{pmatrix} 2k & 0 & 0 \\ 0 & 3k & k \\ 0 & k & 3k \end{pmatrix}.$$

Assuming depolarizing effects are negligible, find how the body will orientate itself if the field is horizontal, in the following circumstances:

(a) the body can rotate freely;

(b) the body is suspended with the $(1,0,0)$ axis vertical;

(c) the body is suspended with the $(0,1,0)$ axis vertical.

26.19 A block of wood contains a number of thin soft-iron nails (of constant permeability). A unit magnetic field directed eastwards induces a magnetic moment in the block having components $(3,1,-2)$, and similar fields directed northwards and vertically upwards induce moments $(1,3,-2)$ and $(-2,-2,2)$ respectively. Show that all the nails lie in parallel planes.

26.20 For tin, the conductivity tensor is diagonal, with entries a, a, and b when referred to its crystal axes. A single crystal is grown in the shape of a long wire of length L and radius r, the axis of the wire making polar angle θ with respect to the crystal's 3-axis. Show that the resistance of the wire is $L(\pi r^2 ab)^{-1}\left(a\cos^2\theta + b\sin^2\theta\right)$.

26.21 By considering an isotropic body subjected to a uniform hydrostatic pressure (no shearing stress), show that the bulk modulus k, defined by the ratio of the pressure to the fractional decrease in volume, is given by $k = E/[3(1-2\sigma)]$ where E is Young's modulus and σ is Poisson's ratio.

26.22 For an isotropic elastic medium under dynamic stress, at time t the displacement u_i and the stress tensor p_{ij} satisfy

$$p_{ij} = c_{ijkl}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right) \qquad \text{and} \qquad \frac{\partial p_{ij}}{\partial x_j} = \rho\frac{\partial^2 u_i}{\partial t^2},$$

where c_{ijkl} is the isotropic tensor given in equation (26.47) and ρ is a constant. Show that both $\nabla\cdot\mathbf{u}$ and $\nabla\times\mathbf{u}$ satisfy wave equations and find the corresponding wave speeds.

26.23 A fourth-order tensor T_{ijkl} has the properties

$$T_{jikl} = -T_{ijkl}, \qquad T_{ijlk} = -T_{ijkl}.$$

Prove that for any such tensor there exists a second-order tensor K_{mn} such that

$$T_{ijkl} = \epsilon_{ijm}\epsilon_{kln}K_{mn}$$

and give an explicit expression for K_{mn}. Consider two (separate) special cases, as follows.

(a) Given that T_{ijkl} is isotropic and $T_{ijji} = 1$, show that T_{ijkl} is uniquely determined and express it in terms of Kronecker deltas.
(b) If now T_{ijkl} has the additional property

$$T_{klij} = -T_{ijkl},$$

show that T_{ijkl} has only three linearly independent components and find an expression for T_{ijkl} in terms of the vector

$$V_i = -\tfrac{1}{4}\epsilon_{jkl}T_{ijkl}.$$

26.24 Working in cylindrical polar coordinates ρ, ϕ, z, parameterise the straight line (geodesic) joining $(1, 0, 0)$ to $(1, \pi/2, 1)$ in terms of s, the distance along the line. Show by substitution that the geodesic equations, derived at the end of section 26.22, are satisfied.

26.25 In a general coordinate system u^i, $i = 1, 2, 3$, in three-dimensional Euclidean space, a volume element is given by

$$dV = |\mathbf{e}_1\, du^1 \cdot (\mathbf{e}_2\, du^2 \times \mathbf{e}_3\, du^3)|.$$

Show that an alternative form for this expression, written in terms of the determinant g of the metric tensor, is given by

$$dV = \sqrt{g}\, du^1\, du^2\, du^3.$$

Show that, under a general coordinate transformation to a new coordinate system u'^i, the volume element dV remains unchanged, i.e. show that it is a scalar quantity.

26.26 By writing down the expression for the square of the infinitesimal arc length $(ds)^2$ in spherical polar coordinates, find the components g_{ij} of the metric tensor in this coordinate system. Hence, using (26.97), find the expression for the divergence of a vector field $\mathbf{v}$ in spherical polars. Calculate the Christoffel symbols (of the second kind) $\Gamma^i{}_{jk}$ in this coordinate system.

26.27 Find an expression for the second covariant derivative $v_{i;\,jk} \equiv (v_{i;\,j})_{;\,k}$ of a vector v_i (see (26.88)). By interchanging the order of differentiation and then subtracting the two expressions, we define the components $R^l{}_{ijk}$ of the *Riemann tensor* as

$$v_{i;\,jk} - v_{i;\,kj} \equiv R^l{}_{ijk}v_l.$$

Show that in a general coordinate system u^i these components are given by

$$R^l{}_{ijk} = \frac{\partial \Gamma^l{}_{ik}}{\partial u^j} - \frac{\partial \Gamma^l{}_{ij}}{\partial u^k} + \Gamma^m{}_{ik}\Gamma^l{}_{mj} - \Gamma^m{}_{ij}\Gamma^l{}_{mk}.$$

By first considering Cartesian coordinates, show that all the components $R^l{}_{ijk} \equiv 0$ for *any* coordinate system in three-dimensional Euclidean space.
In such a space, therefore, we may change the order of the covariant derivatives without changing the resulting expression.

26.28 A curve $\mathbf{r}(t)$ is parameterised by a scalar variable t. Show that the length of the curve between two points, A and B, is given by

$$L = \int_A^B \sqrt{g_{ij}\frac{du^i}{dt}\frac{du^j}{dt}}\,dt.$$

Using the calculus of variations (see chapter 22), show that the curve $\mathbf{r}(t)$ that minimises L satisfies the equation

$$\frac{d^2u^i}{dt^2} + \Gamma^i{}_{jk}\frac{du^j}{dt}\frac{du^k}{dt} = \frac{\ddot{s}}{\dot{s}}\frac{du^i}{dt},$$

where s is the arc length along the curve, $\dot{s} = ds/dt$ and $\ddot{s} = d^2s/dt^2$. Hence, show that if the parameter t is of the form $t = as + b$, where a and b are constants, then we recover the equation for a geodesic (26.101).

[A parameter which, like t, is the sum of a linear transformation of s and a translation is called an *affine* parameter.]

26.29 We may define Christoffel symbols of the first kind by

$$\Gamma_{ijk} = g_{il}\Gamma^l{}_{jk}.$$

Show that these are given by

$$\Gamma_{kij} = \frac{1}{2}\left(\frac{\partial g_{ik}}{\partial u^j} + \frac{\partial g_{jk}}{\partial u^i} - \frac{\partial g_{ij}}{\partial u^k}\right).$$

By permuting indices, verify that

$$\frac{\partial g_{ij}}{\partial u^k} = \Gamma_{ijk} + \Gamma_{jik}.$$

Using the fact that $\Gamma^l{}_{jk} = \Gamma^l{}_{kj}$, show that

$$g_{ij;k} \equiv 0,$$

i.e. that the covariant derivative of the metric tensor is identically zero in all coordinate systems.

26.24 Hints and answers

26.1 (a) $u_1' = x_1\cos(\phi-\theta) - x_2\sin(\phi-\theta)$, etc.;
(b) $u_{11}' = s^2x_1^2 - 2scx_1x_2 + c^2x_2^2 \neq c^2x_2^2 + csx_1x_2 + scx_1x_2 + s^2x_1^2$.

26.3 (a) $(1/\sqrt{2})(\sqrt{2},0,0;0,1,-1;0,1,1)$. (b) $(1/\sqrt{2})(1,0,-1;0,\sqrt{2},0;1,0,1)$.
$\mathbf{r} = (2\sqrt{2},\ -1+\sqrt{2},\ -1-\sqrt{2})^{\mathrm{T}}$.

26.5 Twice contract the array with the outer product of (x,y,z) with itself, thus obtaining the expression $-(x^2+y^2+z^2)^2$, which is an invariant and therefore a scalar.

26.7 Write $A_j(\partial A_i/\partial x_j)$ as $\partial(A_iA_j)/\partial x_j - A_i(\partial A_j/\partial x_j)$.

26.9 (i) Write out the expression for $|\mathsf{A}^{\mathrm{T}}|$, contract both sides of the equation with ϵ_{lmn} and pick out the expression for $|\mathsf{A}|$ on the RHS. Note that $\epsilon_{lmn}\epsilon_{lmn}$ is a numerical scalar.
(iii) Each non-zero term on the RHS contains any particular row index once and only once. The same can be said for the Levi–Civita symbol on the LHS. Thus interchanging two rows is equivalent to interchanging two of the subscripts of ϵ_{lmn}, and thereby reversing its sign. Consequently, the magnitude of $|\mathsf{A}|$ remains the same but its sign is changed.
(v) If, say, $A_{pi} = \lambda A_{pj}$, for some particular pair of values i and j and all p then,

in the (multiple) summation on the RHS, each A_{nk} appears multiplied by (with no summation over i and j)

$$\epsilon_{ijk}A_{li}A_{mj} + \epsilon_{jik}A_{lj}A_{mi} = \epsilon_{ijk}\lambda A_{lj}A_{mj} + \epsilon_{jik}A_{lj}\lambda A_{mj} = 0,$$

since $\epsilon_{ijk} = -\epsilon_{jik}$. Consequently, grouped in this way all terms are zero and $|\mathsf{A}| = 0$.
(vi) Replace A_{mj} by $A_{mj} + \lambda A_{lj}$ and note that $\lambda A_{li}A_{lj}A_{nk}\epsilon_{ijk} = 0$ by virtue of result (v).
(vii) If $\mathsf{C} = \mathsf{AB}$,

$$|\mathsf{C}|\epsilon_{lmn} = A_{lx}B_{xi}A_{my}B_{yj}A_{nz}B_{zk}\epsilon_{ijk}.$$

Contract this with ϵ_{lmn} and show that the RHS is equal to $\epsilon_{xyz}|\mathsf{A}^{\mathrm{T}}|\epsilon_{xyz}|\mathsf{B}|$. It then follows from result (i) that $|\mathsf{C}| = |\mathsf{A}||\mathsf{B}|$.

26.11 $\alpha = |\mathbf{v}|^{-2}$. Note that the most general vector has components $w_i = \lambda v_i + \mu u_i^{(1)} + \nu u_i^{(2)}$, where both $\mathbf{u}^{(1)}$ and $\mathbf{u}^{(2)}$ are orthogonal to $\mathbf{v}$.

26.13 Construct the orthogonal transformation matrix S for the symmetry operation of (say) a rotation of $2\pi/3$ about a body diagonal and, setting $\mathsf{L} = \mathsf{S}^{-1} = \mathsf{S}^{\mathrm{T}}$, construct $\sigma' = \mathsf{L}\sigma\mathsf{L}^{\mathrm{T}}$ and require $\sigma' = \sigma$. Repeat the procedure for (say) a rotation of $\pi/2$ about the x_3-axis. These together show that $\sigma_{11} = \sigma_{22} = \sigma_{33}$ and that all other $\sigma_{ij} = 0$. Further symmetry requirements do not provide any additional constraints.

26.15 The transformation of δ_{ij} has to be included; the principal values are $\pm\mathbf{E}\cdot\mathbf{B}$. The third axis is in the direction $\pm\mathbf{B}\times\mathbf{E}$ with principal value $-|\mathbf{E}|^2$.

26.17 The principal moments give the required ratios.

26.19 The principal permeability, in direction $(1, 1, 2)$, has value 0. Thus all the nails lie in planes to which this is the normal.

26.21 Take $p_{11} = p_{22} = p_{33} = -p$, and $p_{ij} = e_{ij} = 0$ for $i \neq j$, leading to $-p = (\lambda + 2\mu/3)e_{ii}$. The fractional volume change is e_{ii}; λ and μ are as defined in (26.46) and the worked example that follows it.

26.23 Consider $Q_{pq} = \epsilon_{pij}\epsilon_{qkl}T_{ijkl}$ and show that $K_{mn} = Q_{mn}/4$ has the required property.
(a) Argue from the isotropy of T_{ijkl} and ϵ_{ijk} for that of K_{mn} and hence that it must be a multiple of δ_{mn}. Show that the multiplier is uniquely determined and that $T_{ijkl} = (\delta_{il}\delta_{jk} - \delta_{ik}\delta_{jl})/6$.
(b) By relabelling dummy subscripts and using the stated antisymmetry property, show that $K_{nm} = -K_{mn}$. Show that $-2V_i = \epsilon_{min}K_{mn}$ and hence that $K_{mn} = \epsilon_{imn}V_i$. $T_{ijkl} = \epsilon_{kli}V_j - \epsilon_{klj}V_i$.

26.25 Use $|\mathbf{e}_1 \cdot (\mathbf{e}_2 \times \mathbf{e}_3)| = \sqrt{g}$.
Recall that $\sqrt{g'} = |\partial u/\partial u'|\sqrt{g}$ and $du'^1\, du'^2\, du'^3 = |\partial u'/\partial u|\, du^1\, du^2\, du^3$.

26.27 $(v_{i;j})_{;k} = (v_{i;j})_{,k} - \Gamma^l{}_{ik}v_{l;j} - \Gamma^l{}_{jk}v_{i;l}$ and $v_{i;j} = v_{i,j} - \Gamma^m{}_{ij}v_m$. If all components of a tensor equal zero in one coordinate system, then they are zero in all coordinate systems.

26.29 Use $g_{il}g^{ln} = \delta_i^n$ and $g_{ij} = g_{ji}$. Show that

$$g_{ij;k} = \left(\frac{\partial g_{ij}}{\partial u^k} - \Gamma_{jik} - \Gamma_{ijk}\right)\mathbf{e}^i \otimes \mathbf{e}^j$$

and then use the earlier result.

27

Numerical methods

It happens frequently that the end product of a calculation or piece of analysis is one or more algebraic or differential equations, or an integral that cannot be evaluated in closed form or in terms of tabulated or pre-programmed functions. From the point of view of the physical scientist or engineer, who needs numerical values for prediction or comparison with experiment, the calculation or analysis is thus incomplete.

With the ready availability of standard packages on powerful computers for the numerical solution of equations, both algebraic and differential, and for the evaluation of integrals, in principle there is no need for the investigator to do anything other than turn to them. However, it should be a part of every engineer's or scientist's repertoire to have some understanding of the kinds of procedure that are being put into practice within those packages. The present chapter indicates (at a simple level) some of the ways in which analytically intractable problems can be tackled using numerical methods.

In the restricted space available in a book of this nature, it is clearly not possible to give anything like a full discussion, even of the elementary points that will be made in this chapter. The limited objective adopted is that of explaining and illustrating by simple examples some of the basic principles involved. In many cases, the examples used can be solved in closed form anyway, but this 'obviousness' of the answers should not detract from their illustrative usefulness, and it is hoped that their transparency will help the reader to appreciate some of the inner workings of the methods described.

The student who proposes to study complicated sets of equations or make repeated use of the same procedures by, for example, writing computer programs to carry out the computations, will find it essential to acquire a good understanding of topics hardly mentioned here. Amongst these are the sensitivity of the adopted procedures to errors introduced by the limited accuracy with which a numerical value can be stored in a computer (rounding errors) and to the

errors introduced as a result of approximations made in setting up the numerical procedures (truncation errors). For this scale of application, books specifically devoted to numerical analysis, data analysis and computer programming should be consulted.

So far as is possible, the method of presentation here is that of indicating and discussing in a qualitative way the main steps in the procedure, and then of following this with an elementary worked example. The examples have been restricted in complexity to a level at which they can be carried out with a pocket calculator. Naturally it will not be possible for the student to check all the numerical values presented, unless he or she has a programmable calculator or computer readily available, and even then it might be tedious to do so. However, it is advisable to check the initial step and at least one step in the middle of each repetitive calculation given in the text, so that how the symbolic equations are used with actual numbers is understood. Clearly the intermediate step should be chosen to be at a point in the calculation at which the changes are still sufficiently large that they can be detected by whatever calculating device is used.

Where alternative methods for solving the same type of problem are discussed, for example in finding the roots of a polynomial equation, we have usually taken the same example to illustrate each method. This could give the mistaken impression that the methods are very restricted in applicability, but it is felt by the authors that using the same examples repeatedly has sufficient advantages, in terms of illustrating the *relative* characteristics of competing methods, to justify doing so. Once the principles are clear, little is to be gained by using new examples each time, and, in fact, having some prior knowledge of the 'correct answer' should allow the reader to judge the efficiency and dangers of particular methods as the successive steps are followed through.

One other point remains to be mentioned. Here, in contrast with every other chapter of this book, the value of a large selection of exercises is not clear cut. The reader with sufficient computing resources to tackle them can easily devise algebraic or differential equations to be solved, or functions to be integrated (which perhaps have arisen in other contexts). Further, the solutions of these problems will be self-checking, for the most part. Consequently, although a number of exercises are included, no attempt has been made to test the full range of ideas treated in this chapter.

27.1 Algebraic and transcendental equations

The problem of finding the real roots of an equation of the form $f(x) = 0$, where $f(x)$ is an algebraic or transcendental function of x, is one that can sometimes be treated numerically, even if explicit solutions in closed form are not feasible.

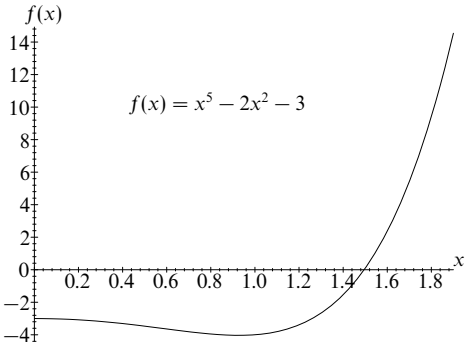


Figure 27.1 A graph of the function $f(x) = x^5 - 2x^2 - 3$ for x in the range $0 \leq x \leq 1.9$.

Examples of the types of equation mentioned are the quartic equation,

$$ax^4 + bx + c = 0,$$

and the transcendental equation,

$$x - 3\tanh x = 0.$$

The latter type is characterised by the fact that it contains, in effect, a polynomial of infinite order on the LHS.

We will discuss four methods that, in various circumstances, can be used to obtain the real roots of equations of the above types. In all cases we will take as the specific equation to be solved the fifth-order polynomial equation

$$f(x) \equiv x^5 - 2x^2 - 3 = 0. \tag{27.1}$$

The reasons for using the same equation each time were discussed in the introduction to this chapter.

For future reference, and so that the reader may follow some of the calculations leading to the evaluation of the real root of (27.1), a graph of $f(x)$ in the range $0 \leq x \leq 1.9$ is shown in figure 27.1.

Equation (27.1) is one for which no solution can be found in closed form, that is in the form $x = a$, where a does not explicitly contain x. The general scheme to be employed will be an iterative one in which successive approximations to a real root of (27.1) will be obtained, each approximation, it is to be hoped, being better than the preceding one; certainly, we require that the approximations converge and that they have as their limit the sought-for root. Let us denote the required

root by ξ and the values of successive approximations by $x_1, x_2, \ldots, x_n, \ldots$. Then, for any particular method to be successful,

$$\lim_{n\to\infty} x_n = \xi, \qquad \text{where } f(\xi) = 0. \tag{27.2}$$

However, success as defined here is not the only criterion. Since, in practice, only a finite number of iterations will be possible, it is important that the values of x_n be close to that of ξ for all $n > N$, where N is a relatively low number; exactly how low it is naturally depends on the computing resources available and the accuracy required in the final answer.

So that the reader may assess the progress of the calculations that follow, we record that to nine significant figures the real root of equation (27.1) has the value

$$\xi = 1.495\,106\,40. \tag{27.3}$$

We now consider in turn four methods for determining the value of this root.

27.1.1 Rearrangement of the equation

If equation (27.1), $f(x) = 0$, can be recast into the form

$$x = \phi(x), \tag{27.4}$$

where $\phi(x)$ is a *slowly* varying function of x, then an iteration scheme

$$x_{n+1} = \phi(x_n) \tag{27.5}$$

will often produce a fair approximation to the root ξ after a few iterations, as follows. Clearly, $\xi = \phi(\xi)$, since $f(\xi) = 0$; thus, when x_n is close to ξ, the next approximation, x_{n+1}, will differ little from x_n, the actual size of the difference giving an order-of-magnitude indication of the inaccuracy in x_{n+1} (when compared with ξ).

In the present case, the equation can be written

$$x = (2x^2 + 3)^{1/5}. \tag{27.6}$$

Because of the presence of the one-fifth power, the RHS is rather insensitive to the value of x used to compute it, and so the form (27.6) fits the general requirements for the method to work satisfactorily. It remains only to choose a starting approximation. It is easy to see from figure 27.1 that the value $x = 1.5$ would be a good starting point, but, so that the behaviour of the procedure at values some way from the actual root can be studied, we will make a poorer choice, $x_1 = 1.7$.

With this starting value and the general recurrence relationship

$$x_{n+1} = (2x_n^2 + 3)^{1/5}, \tag{27.7}$$

n	x_n	$f(x_n)$
1	1.7	5.42
2	1.544 18	1.01
3	1.506 86	2.28×10^{-1}
4	1.497 92	5.37×10^{-2}
5	1.495 78	1.28×10^{-2}
6	1.495 27	3.11×10^{-3}
7	1.495 14	7.34×10^{-4}
8	1.495 12	1.76×10^{-4}

Table 27.1 Successive approximations to the root of (27.1) using the method of rearrangement.

n	A_n	$f(A_n)$	B_n	$f(B_n)$	x_n	$f(x_n)$
1	1.0	−4.0000	1.7	5.4186	1.2973	−2.6916
2	1.2973	−2.6916	1.7	5.4186	1.4310	−1.0957
3	1.4310	−1.0957	1.7	5.4186	1.4762	−0.3482
4	1.4762	−0.3482	1.7	5.4186	1.4897	−0.1016
5	1.4897	−0.1016	1.7	5.4186	1.4936	−0.0289
6	1.4936	−0.0289	1.7	5.4186	1.4947	−0.0082

Table 27.2 Successive approximations to the root of (27.1) using linear interpolation.

successive values can be found. These are recorded in table 27.1. Although not strictly necessary, the value of $f(x_n) \equiv x_n^5 - 2x_n^2 - 3$ is also shown at each stage.

It will be seen that x_7 and all later x_n agree with the precise answer (27.3) to within one part in 10^4. However, $f(x_n)$ and $x_n - \xi$ are both reduced by a factor of only about 4 for each iteration; thus a large number of iterations would be needed to produce a very accurate answer. The factor 4 is, of course, specific to this particular problem and would be different for a different equation. The successive values of x_n are shown in graph (a) of figure 27.2.

27.1.2 Linear interpolation

In this approach two values, A_1 and B_1, of x are chosen with $A_1 < B_1$ and such that $f(A_1)$ and $f(B_1)$ have opposite signs. The chord joining the two points $(A_1, f(A_1))$ and $(B_1, f(B_1))$ is then notionally constructed, as illustrated in graph (b) of figure 27.2, and the value x_1 at which the chord cuts the x-axis is determined by the *interpolation formula*

$$x_n = \frac{A_n f(B_n) - B_n f(A_n)}{f(B_n) - f(A_n)}, \tag{27.8}$$

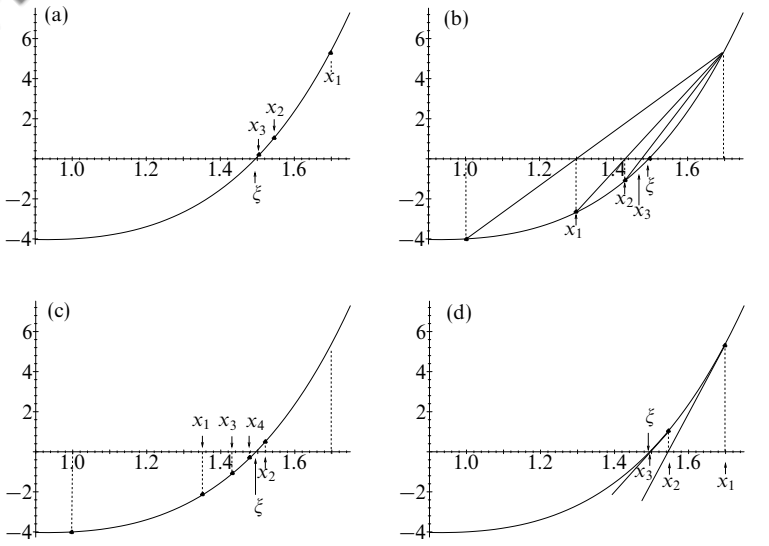


Figure 27.2 Graphical illustrations of the iteration methods discussed in the text: (a) rearrangement; (b) linear interpolation; (c) binary chopping; (d) Newton–Raphson.

with $n = 1$. Next, $f(x_1)$ is evaluated and the process repeated after replacing either A_1 or B_1 by x_1, according to whether $f(x_1)$ has the same sign as $f(A_1)$ or $f(B_1)$, respectively. In figure 27.2(b), A_1 is the one replaced.

As can be seen in the particular example that we are considering, with this method there is a tendency, if the curvature of $f(x)$ is of constant sign near the root, for one of the two ends of the successive chords to remain unchanged.

Starting with the initial values $A_1 = 1$ and $B_1 = 1.7$, the results of the first five iterations using (27.8) are given in table 27.2 and indicated in graph (b) of figure 27.2. As with the rearrangement method, the improvement in accuracy, as measured by $f(x_n)$ and $x_n - \xi$, is a fairly constant factor at each iteration (approximately 3 in this case), and for our particular example there is little to choose between the two. Both tend to their limiting value of ξ monotonically, from either higher or lower values, and this makes it difficult to estimate limits within which ξ can safely be presumed to lie. The next method to be described gives at any stage a range of values within which ξ is *known* to lie.

n	A_n	$f(A_n)$	B_n	$f(B_n)$	x_n	$f(x_n)$
1	1.0000	−4.0000	1.7000	5.4186	1.3500	−2.1610
2	1.3500	−2.1610	1.7000	5.4186	1.5250	0.5968
3	1.3500	−2.1610	1.5250	0.5968	1.4375	−0.9946
4	1.4375	−0.9946	1.5250	0.5968	1.4813	−0.2573
5	1.4813	−0.2573	1.5250	0.5968	1.5031	0.1544
6	1.4813	−0.2573	1.5031	0.1544	1.4922	−0.0552
7	1.4922	−0.0552	1.5031	0.1544	1.4977	0.0487
8	1.4922	−0.0552	1.4977	0.0487	1.4949	−0.0085

Table 27.3 Successive approximations to the root of (27.1) using binary chopping.

27.1.3 Binary chopping

Again two values of x, A_1 and B_1, that straddle the root are chosen, such that $A_1 < B_1$ and $f(A_1)$ and $f(B_1)$ have opposite signs. The interval between them is then halved by forming

$$x_n = \tfrac{1}{2}(A_n + B_n), \tag{27.9}$$

with $n = 1$, and $f(x_1)$ is evaluated. It should be noted that x_1 is determined solely by A_1 and B_1, and not by the values of $f(A_1)$ and $f(B_1)$ as in the linear interpolation method. Now x_1 is used to replace either A_1 or B_1, depending on which of $f(A_1)$ or $f(B_1)$ has the same sign as $f(x_1)$, i.e. if $f(A_1)$ and $f(x_1)$ have the same sign then x_1 replaces A_1. The process isthen repeated to obtain x_2, x_3, etc.

This has been carried through in table 27.3 for our standard equation (27.1) and is illustrated in figure 27.2(c). The entries have been rounded to four places of decimals. It is suggested that the reader follows through the sequential replacements of the A_n and B_n in the table and correlates the first few of these with graph (c) of figure 27.2.

Clearly, the accuracy with which ξ is known in this approach increases by only a factor of 2 at each step, but this accuracy is predictable at the outset of the calculation and (unless $f(x)$ has very violent behaviour near $x = \xi$) a range of x in which ξ lies can be safely stated at any stage. At the stage reached in the last row of table 27.3 it may be stated that $1.4949 < \xi < 1.4977$. Thus binary chopping gives a simple approximation method (it involves less multiplication than linear interpolation, for example) that is predictable and relatively safe, although its convergence is slow.

27.1.4 Newton–Raphson method

The Newton–Raphson (NR) procedure is somewhat similar to the interpolation method, but, as will be seen, has one distinct advantage over the latter. Instead

n	x_n	$f(x_n)$
1	1.7	5.42
2	1.545 01	1.03
3	1.498 87	7.20×10^{-2}
4	1.495 13	4.49×10^{-4}
5	1.495 106 40	2.6×10^{-8}
6	1.495 106 40	—

Table 27.4 Successive approximations to the root of (27.1) using the Newton–Raphson method.

of (notionally) constructing the chord between two points on the curve of $f(x)$ against x, the tangent to the curve is notionally constructed at each successive value of x_n, and the next value, x_{n+1}, is taken as the point at which the tangent cuts the axis $f(x) = 0$. This is illustrated in graph (d) of figure 27.2.

If the nth value is x_n, the tangent to the curve of $f(x)$ at that point has slope $f'(x_n)$ and passes through the point $x = x_n$, $y = f(x_n)$. Its equation is thus

$$y(x) = (x - x_n)f'(x_n) + f(x_n). \tag{27.10}$$

The value of x at which $y = 0$ is then taken as x_{n+1}; thus the condition $y(x_{n+1}) = 0$ yields, from (27.10), the iteration scheme

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}. \tag{27.11}$$

This is the *Newton–Raphson iteration formula*. Clearly, if x_n is close to ξ then x_{n+1} is close to x_n, as it should be. It is also apparent that if any of the x_n comes close to a stationary point of f, so that $f'(x_n)$ is close to zero, the scheme is not going to work well.

For our standard example, (27.11) becomes

$$x_{n+1} = x_n - \frac{x_n^5 - 2x_n^2 - 3}{5x_n^4 - 4x_n} = \frac{4x_n^5 - 2x_n^2 + 3}{5x_n^4 - 4x_n}. \tag{27.12}$$

Again taking a starting value of $x_1 = 1.7$, we obtain in succession the entries in table 27.4. The different values are given to an increasing number of decimal places as the calculation proceeds; $f(x_n)$ is also recorded.

It is apparent that this method is unlike the previous ones in that the increase in accuracy of the answer is not constant throughout the iterations but improves dramatically as the required root is approached. Away from the root the behaviour of the series is less satisfactory, and from its geometrical interpretation it can be seen that if, for example, there were a maximum or minimum near the root then the series could oscillate between values on either side of it (instead of 'homing in' on the root). The reason for the good convergence near the root is discussed in the next section.

Of the four methods mentioned, no single one is ideal, and, in practice, some mixture of them is usually to be preferred. The particular combination of methods selected will depend a great deal on how easily the progress of the calculation may be monitored, but some combination of the first three methods mentioned, followed by the NR scheme if great accuracy were required, would be suitable for most situations.

27.2 Convergence of iteration schemes

For iteration schemes in which x_{n+1} can be expressed as a differentiable function of x_n, for example the rearrangement or NR methods of the previous section, a partial analysis of the conditions necessary for a successful scheme can be made as follows.

Suppose the general iteration formula is expressed as

$$x_{n+1} = F(x_n) \tag{27.13}$$

((27.7) and (27.12) are examples). Then the sequence of values $x_1, x_2, \ldots, x_n, \ldots$ is required to converge to the value ξ that satisfies both

$$f(\xi) = 0 \qquad \text{and} \qquad \xi = F(\xi). \tag{27.14}$$

If the error in the solution at the nth stage is ϵ_n, i.e. $x_n = \xi + \epsilon_n$, then

$$\xi + \epsilon_{n+1} = x_{n+1} = F(x_n) = F(\xi + \epsilon_n). \tag{27.15}$$

For the iteration process to converge, a decreasing error is required, i.e. $|\epsilon_{n+1}| < |\epsilon_n|$. To see what this implies about F, we expand the right-hand term of (27.15) by means of a Taylor series and use (27.14) to replace (27.15) by

$$\xi + \epsilon_{n+1} = \xi + \epsilon_n F'(\xi) + \tfrac{1}{2}\epsilon_n^2 F''(\xi) + \cdots . \tag{27.16}$$

This shows that, for small ϵ_n,

$$\epsilon_{n+1} \approx F'(\xi)\epsilon_n$$

and that a necessary (but not sufficient) condition for convergence is that

$$|F'(\xi)| < 1. \tag{27.17}$$

It should be noted that this is a condition on $F'(\xi)$ and not on $f'(\xi)$, which may have any finite value. Figure 27.3 illustrates in a graphical way how the convergence proceeds for the case $0 < F'(\xi) < 1$.

Equation (27.16) suggests that if $F(x)$ can be chosen so that $F'(\xi) = 0$ then the ratio $|\epsilon_{n+1}/\epsilon_n|$ could be made very small, of order ϵ_n in fact. To go even further, if it can be arranged that the first few derivatives of F vanish at $x = \xi$ then the

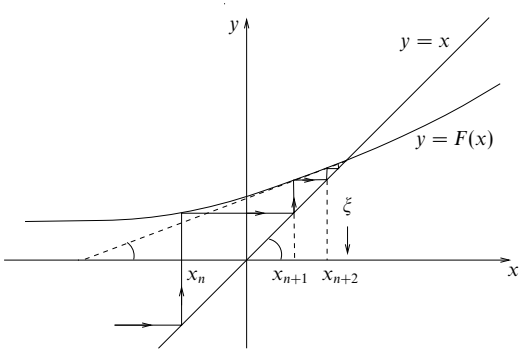


Figure 27.3 Illustration of the convergence of the iteration scheme $x_{n+1} = F(x_n)$ when $0 < F'(\xi) < 1$, where $\xi = F(\xi)$. The line $y = x$ makes an angle $\pi/4$ with the axes. The broken line makes an angle $\tan^{-1} F'(\xi)$ with the x-axis.

convergence, once x_n has become close to ξ, could be very rapid indeed. If the first $N-1$ derivatives of F vanish at $x = \xi$, i.e.

$$F'(\xi) = F''(\xi) = \cdots = F^{(N-1)}(\xi) = 0 \tag{27.18}$$

and consequently

$$\epsilon_{n+1} = \mathrm{O}(\epsilon_n^N), \tag{27.19}$$

then the scheme is said to have *Nth-order convergence*.

This is the explanation of the significant difference in convergence between the NR scheme and the others discussed (judged by reference to (27.19), so that the differentiability of the function F is not a prerequisite). The NR procedure has second-order convergence, as is shown by the following analysis. Since

$$\begin{aligned} F(x) &= x - \frac{f(x)}{f'(x)}, \\ F'(x) &= 1 - \frac{f'(x)}{f'(x)} + \frac{f(x)f''(x)}{[f'(x)]^2} \\ &= \frac{f(x)f''(x)}{[f'(x)]^2}. \end{aligned}$$

Now, provided $f'(\xi) \neq 0$, it follows that $F'(\xi) = 0$ because $f(x) = 0$ at $x = \xi$.

n	x_{n+1}	ϵ_n
1	8.5	4.5
2	5.191	1.19
3	4.137	1.4×10^{-1}
4	4.002 257	2.3×10^{-3}
5	4.000 000 637	6.4×10^{-7}
6	4	—

Table 27.5 Successive approximations to $\sqrt{16}$ using the iteration scheme (27.20).

► *The following is an iteration scheme for finding the square root of X:*

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{X}{x_n}\right). \tag{27.20}$$

Show that it has second-order convergence and illustrate its efficiency by finding, say, $\sqrt{16}$ starting with a very poor guess, $\sqrt{16} = 1$.

If this scheme does converge to ξ then ξ will satisfy

$$\xi = \frac{1}{2}\left(\xi + \frac{X}{\xi}\right) \quad \Rightarrow \quad \xi^2 = X,$$

as required. The iteration function F is given by

$$F(x) = \frac{1}{2}\left(x + \frac{X}{x}\right),$$

and so, since $\xi^2 = X$,

$$F'(\xi) = \frac{1}{2}\left(1 - \frac{X}{x^2}\right)_{x=\xi} = 0,$$

whilst

$$F''(\xi) = \left(\frac{X}{x^3}\right)_{x=\xi} = \frac{1}{\xi} \neq 0.$$

Thus the procedure has second-order, but not third-order, convergence.

We now show the procedure in action. Table 27.5 gives successive values of x_n and of ϵ_n, the difference between x_n and the true value, 4. As we can see, the scheme is crude initially, but once x_n gets close to ξ, it homes in on the true value extremely rapidly. ◄

27.3 Simultaneous linear equations

As we saw in chapter 8, many situations in physical science can be described approximately or exactly by a set of N simultaneous linear equations in N

variables (unknowns), x_i, $i = 1, 2, \ldots, N$. The equations take the general form

$$\begin{aligned} A_{11}x_1 + A_{12}x_2 + \cdots + A_{1N}x_N &= b_1, \\ A_{21}x_1 + A_{22}x_2 + \cdots + A_{2N}x_N &= b_2, \\ &\vdots \\ A_{N1}x_1 + A_{N2}x_2 + \cdots + A_{NN}x_N &= b_N, \end{aligned} \tag{27.21}$$

where the A_{ij} are constants and form the elements of a square matrix A. The b_i are given and form a column matrix b. If A is non-singular then (27.21) can be solved for the x_i using the inverse of A, according to the formula

$$\mathsf{x} = \mathsf{A}^{-1}\mathsf{b}.$$

This approach was discussed at length in chapter 8 and will not be considered further here.

27.3.1 Gaussian elimination

We follow instead a continuation of one of the earliest techniques acquired by a student of algebra, namely the solving of simultaneous equations (initially only two in number) by the successive elimination of all the variables but one. This (known as *Gaussian elimination*) is achieved by using, at each stage, one of the equations to obtain an explicit expression for one of the remaining x_i in terms of the others and then substituting for that x_i in all other remaining equations. Eventually a single linear equation in just one of the unknowns is obtained. This is then solved and the result is resubstituted in previously derived equations (in reverse order) to establish values for all the x_i.

This method is probably very familiar to the reader, and so a specific example to illustrate this alone seems unnecessary. Instead, we will show how a calculation along such lines might be arranged so that the errors due to the inherent lack of precision in any calculating equipment do not become excessive. This can happen if the value of N is large and particularly (and we will merely state this) if the elements $A_{11}, A_{22}, \ldots, A_{NN}$ on the leading diagonal of the matrix in (27.21) are small compared with the off-diagonal elements.

The process to be described is known as *Gaussian elimination with interchange*. The only, but essential, difference from straightforward elimination is that before each variable x_i is eliminated, the equations are reordered to put the largest (in modulus) remaining coefficient of x_i on the leading diagonal.

We will take as an illustration a straightforward three-variable example, which can in fact be solved perfectly well without any interchange since, with simple numbers and only two eliminations to perform, rounding errors do not have a chance to build up. However, the important thing is that the reader should

appreciate how this would apply in (say) a computer program for a 1000-variable case, perhaps with unforseeable zeros or very small numbers appearing on the leading diagonal.

►*Solve the simultaneous equations*

$$\begin{array}{lrrrcl} \text{(a)} & x_1 & +6x_2 & -4x_3 & = & 8, \\ \text{(b)} & 3x_1 & -20x_2 & +x_3 & = & 12, \\ \text{(c)} & -x_1 & +3x_2 & +5x_3 & = & 3. \end{array} \tag{27.22}$$

Firstly, we interchange rows (a) and (b) to bring the term $3x_1$ onto the leading diagonal. In the following, we label the important equations (I), (II), (III), and the others alphabetically. A general (i.e. variable) label will be denoted by j.

$$\begin{array}{lrrrcl} \text{(I)} & 3x_1 & -20x_2 & +x_3 & = & 12, \\ \text{(d)} & x_1 & +6x_2 & -4x_3 & = & 8, \\ \text{(e)} & -x_1 & +3x_2 & +5x_3 & = & 3. \end{array}$$

For $(j) =$ (d) and (e), replace row (j) by

$$\text{row } (j) - \frac{a_{j1}}{3} \times \text{row (I)},$$

where a_{j1} is the coefficient of x_1 in row (j), to give the two equations

$$\text{(II)} \quad \left(6 + \tfrac{20}{3}\right) x_2 + \left(-4 - \tfrac{1}{3}\right) x_3 = 8 - \tfrac{12}{3},$$

$$\text{(f)} \quad \left(3 - \tfrac{20}{3}\right) x_2 + \left(5 + \tfrac{1}{3}\right) x_3 = 3 + \tfrac{12}{3}.$$

Now $|6 + \frac{20}{3}| > |3 - \frac{20}{3}|$ and so no interchange is required before the next elimination. To eliminate x_2, replace row (f) by

$$\text{row (f)} - \frac{\left(-\frac{11}{3}\right)}{\frac{38}{3}} \times \text{row (II)}.$$

This gives

$$\text{(III)} \qquad \left[\tfrac{16}{3} + \tfrac{11}{38} \times \tfrac{(-13)}{3}\right] x_3 = 7 + \tfrac{11}{38} \times 4.$$

Collecting together and tidying up the final equations, we have

$$\begin{array}{lrrrcl} \text{(I)} & 3x_1 & -20x_2 & +x_3 & = & 12, \\ \text{(II)} & & 38x_2 & -13x_3 & = & 12, \\ \text{(III)} & & & x_3 & = & 2. \end{array}$$

Starting with (III) and working backwards, it is now a simple matter to obtain

$$x_1 = 10, \qquad x_2 = 1, \qquad x_3 = 2. \text{ ◄}$$

27.3.2 Gauss–Seidel iteration

In the example considered in the previous subsection an explicit way of solving a set of simultaneous equations was given, the accuracy obtainable being limited only by the rounding errors in the calculating facilities available, and the calculation was planned to minimise these. However, in some situations it may be that only an approximate solution is needed. If, for a large number of variables, this is

the case then an iterative method may produce a satisfactory degree of precision with less calculation. Such a method, known as *Gauss–Seidel iteration*, is based upon the following analysis.

The problem is again that of finding the components of the column matrix x that satisfies

$$\mathsf{Ax} = \mathsf{b} \tag{27.23}$$

when A and b are a given matrix and column matrix, respectively.

The steps of the Gauss–Seidel scheme are as follows.

(i) Rearrange the equations (usually by simple division on both sides of each equation) so that all diagonal elements of the new matrix C are unity, i.e. (27.23) becomes

$$\mathsf{Cx} = \mathsf{d}, \tag{27.24}$$

where $\mathsf{C} = \mathsf{I} - \mathsf{F}$, and F has zeros as its diagonal elements.

(ii) Step (i) produces

$$\mathsf{Fx} + \mathsf{d} = \mathsf{Ix} = \mathsf{x}, \tag{27.25}$$

and this forms the basis of an iteration scheme,

$$\mathsf{x}_{n+1} = \mathsf{Fx}_n + \mathsf{d}, \tag{27.26}$$

where x_n is the nth approximation to the required solution vector $\boldsymbol{\xi}$.

(iii) To improve the convergence, the matrix F, which has zeros on its leading diagonal, can be written as the sum of two matrices L and U that have non-zero elements only below and above the leading diagonal, respectively:

$$\mathsf{L}_{ij} = \begin{cases} \mathsf{F}_{ij} & \text{if } i > j, \\ 0 & \text{otherwise,} \end{cases}$$
$$\mathsf{U}_{ij} = \begin{cases} \mathsf{F}_{ij} & \text{if } i < j, \\ 0 & \text{otherwise.} \end{cases} \tag{27.27}$$

This allows the latest values of the components of x to be used at each stage and an improved form of (27.26) to be obtained:

$$\mathsf{x}_{n+1} = \mathsf{Lx}_{n+1} + \mathsf{Ux}_n + \mathsf{d}. \tag{27.28}$$

To see why this is possible, we note, for example, that when calculating, say, the fourth component of x_{n+1}, its first three components are already known, and, because of the structure of L, these are the only ones needed to evaluate the fourth component of Lx_{n+1}.

n	x_1	x_2	x_3
1	2	2	2
2	4	0.1	1.34
3	12.76	1.381	2.323
4	9.008	0.867	1.881
5	10.321	1.042	2.039
6	9.902	0.987	1.988
7	10.029	1.004	2.004

Table 27.6 Successive approximations to the solution of simultaneous equations (27.29) using the Gauss–Seidel iteration method.

►*Obtain an approximate solution to the simultaneous equations*

$$\begin{aligned} x_1 \quad +6x_2 \quad -4x_3 &= 8, \\ 3x_1 \quad -20x_2 \quad +x_3 &= 12, \\ -x_1 \quad +3x_2 \quad +5x_3 &= 3. \end{aligned} \tag{27.29}$$

These are the same equations as were solved in subsection 27.3.1.

Divide the equations by 1, −20 and 5, respectively, to give

$$\begin{aligned} x_1 + 6x_2 - 4x_3 &= 8, \\ -0.15x_1 + x_2 - 0.05x_3 &= -0.6, \\ -0.2x_1 + 0.6x_2 + x_3 &= 0.6. \end{aligned}$$

Thus, set out in matrix form, (27.28) is, in this case, given by

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}_{n+1} = \begin{pmatrix} 0 & 0 & 0 \\ 0.15 & 0 & 0 \\ 0.2 & -0.6 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}_{n+1} + \begin{pmatrix} 0 & -6 & 4 \\ 0 & 0 & 0.05 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}_{n} + \begin{pmatrix} 8 \\ -0.6 \\ 0.6 \end{pmatrix}.$$

Suppose initially ($n = 1$) we guess each component to have the value 2. Then the successive sets of values of the three quantities generated by this scheme are as shown in table 27.6. Even with the rather poor initial guess, a close approximation to the exact result, $x_1 = 10$, $x_2 = 1$, $x_3 = 2$, is obtained in only a few iterations. ◄

27.3.3 Tridiagonal matrices

Although for the solution of most matrix equations $\mathsf{Ax} = \mathsf{b}$ the number of operations required increases rapidly with the size $N \times N$ of the matrix (roughly as N^3), for one particularly simple kind of matrix the computing required increases only linearly with N. This type often occurs in physical situations in which objects in an ordered set interact only with their nearest neighbours and is one in which only the leading diagonal and the diagonals immediately above and below it

contain non-zero entries. Such matrices are known as tridiagonal matrices. They may also be used in numerical approximations to the solutions of certain types of differential equation.

A typical matrix equation involving a tridiagonal matrix is as follows:

$$\begin{pmatrix} b_1 & c_1 & & & & 0 \\ a_2 & b_2 & c_2 & & & \\ & a_3 & b_3 & c_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & a_{N-1} & b_{N-1} & c_{N-1} \\ 0 & & & & a_N & b_N \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{N-1} \\ x_N \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{N-1} \\ y_N \end{pmatrix} \tag{27.30}$$

So as to keep the entries in the matrix as free from subscripts as possible, we have used a, b and c to indicate subdiagonal, leading diagonal and superdiagonal elements, respectively. As a consequence, we have had to change the notation for the column matrix on the RHS from b to (say) y.

In such an equation the first and last rows involve x_1 and x_N, respectively, and so the solution could be found by letting x_1 be unknown and then solving in turn each row of the equation in terms of x_1, and finally determining x_1 by requiring the next-to-last line to generate for x_N an equation compatible with that given by the last line. However, if the matrix is large this becomes a very cumbersome operation, and a simpler method is to assume a form of solution

$$x_{i-1} = \theta_{i-1}x_i + \phi_{i-1}. \tag{27.31}$$

Since the ith line of the matrix equation is

$$a_i x_{i-1} + b_i x_i + c_i x_{i+1} = y_i,$$

we must have, by substituting for x_{i-1}, that

$$(a_i\theta_{i-1} + b_i)x_i + c_i x_{i+1} = y_i - a_i\phi_{i-1}.$$

This is also in the form of (27.31), but with i replaced by $i+1$. Thus the recurrence formulae for θ_i and ϕ_i are

$$\theta_i = \frac{-c_i}{a_i\theta_{i-1} + b_i}, \qquad \phi_i = \frac{y_i - a_i\phi_{i-1}}{a_i\theta_{i-1} + b_i}, \tag{27.32}$$

provided the denominator does not vanish for any i. From the first of the matrix equations it follows that $\theta_1 = -c_1/b_1$ and $\phi_1 = y_1/b_1$. The equations may now be solved for the x_i in two stages without carrying through an unknown quantity. First, all the θ_i and ϕ_i are generated using (27.32) and the values of θ_1 and ϕ_1, then, as a second stage, (27.31) is used to evaluate the x_i, starting with x_N $(= \phi_N)$ and working backwards.

►*Solve the following tridiagonal matrix equation, in which only non-zero elements are shown:*

$$\begin{pmatrix} 1 & 2 & & & & \\ -1 & 2 & 1 & & & \\ & 2 & -1 & 2 & & \\ & & 3 & 1 & 1 & \\ & & & 3 & 4 & 2 \\ & & & & -2 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} = \begin{pmatrix} 4 \\ 3 \\ -3 \\ 10 \\ 7 \\ -2 \end{pmatrix}. \tag{27.33}$$

The solution is set out in table 27.7, in which the arrows indicate the general flow of the calculation. First, the columns of a_i, b_i, c_i and y_i are filled in from the original equation (27.33) and then the recurrence relations (27.32) are used to fill in the successive rows starting at the top; on each row we work from left to right as far as and including the ϕ_i column. Finally, the bottom entry in the the x_i column is set equal to the bottom entry in the completed ϕ_i column and the rest of the x_i column is completed by using (27.31) and working up from the bottom. Thus the solution is $x_1 = 2$; $x_2 = 1$; $x_3 = 3$; $x_4 = -1$; $x_5 = 2$; $x_6 = 1$. ◄

	a_i	b_i	c_i		$a_i\theta_{i-1} + b_i$	θ_i	y_i	$a_i\phi_{i-1}$	ϕ_i	x_i	
↓	0	1	2	→	1	−2	4	0	4	2	↑
↓	−1	2	1	→	4	−1/4	3	−4	7/4	1	↑
↓	2	−1	2	→	−3/2	4/3	−3	7/2	13/3	3	↑
↓	3	1	1	→	5	−1/5	10	13	−3/5	−1	↑
↓	3	4	2	→	17/5	−10/17	7	−9/5	44/17	2	↑
↓	−2	2	0	→	54/17	0	−2	−88/17	1 →	1	↑

Table 27.7 The solution of tridiagonal matrix equation (27.33). The arrows indicate the general flow of the calculation, as described in the text.

27.4 Numerical integration

As noted at the start of this chapter, with modern computers and computer packages – some of which will present solutions in algebraic form, where that is possible – the inability to find a closed-form expression for an integral no longer presents a problem. But, just as for the solution of algebraic equations, it is extremely important that scientists and engineers should have some idea of the procedures on which such packages are based. In this section we discuss some of the more elementary methods used to evaluate integrals numerically and at the same time indicate the basis of more sophisticated procedures.

The standard integral evaluation has the form

$$I = \int_a^b f(x)\,dx, \tag{27.34}$$

where the integrand $f(x)$ may be given in analytic or tabulated form, but for the cases under consideration no closed-form expression for I can be obtained. All

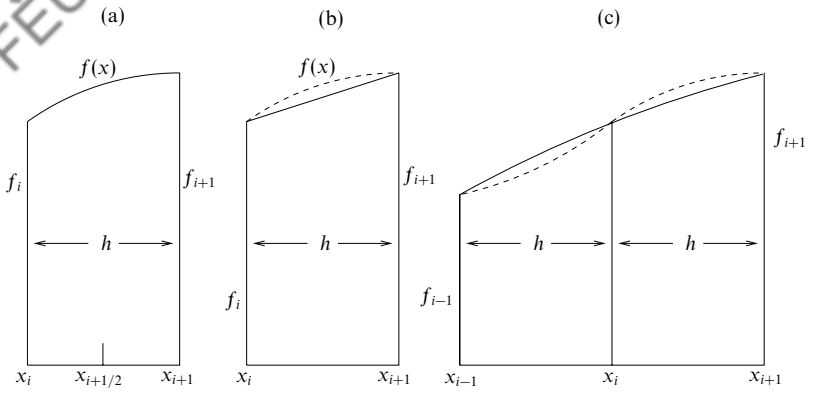


Figure 27.4 (a) Definition of nomenclature. (b) The approximation in using the trapezium rule; $f(x)$ is indicated by the broken curve. (c) Simpson's rule approximation; $f(x)$ is indicated by the broken curve. The solid curve is part of the approximating parabola.

numerical evaluations of I are based on regarding I as the area under the curve of $f(x)$ between the limits $x = a$ and $x = b$ and attempting to estimate that area.

The simplest methods of doing this involve dividing up the interval $a \le x \le b$ into N equal sections, each of length $h = (b - a)/N$. The dividing points are labelled x_i, with $x_0 = a$, $x_N = b$, i running from 0 to N. The point x_i is a distance ih from a. The central value of x in a strip ($x = x_i + h/2$) is denoted for brevity by $x_{i+1/2}$, and for the same reason $f(x_i)$ is written as f_i. This nomenclature is indicated graphically in figure 27.4(a).

So that we may compare later estimates of the area under the curve with the true value, we next obtain an exact expression for I, even though we cannot evaluate it. To do this we need to consider only one strip, say that between x_i and x_{i+1}. For this strip the area is, using Taylor's expansion,

$$\begin{aligned}\int_{-h/2}^{h/2} f(x_{i+1/2}+y)\,dy &= \int_{-h/2}^{h/2} \sum_{n=0}^{\infty} f^{(n)}(x_{i+1/2})\frac{y^n}{n!}\,dy \\ &= \sum_{n=0}^{\infty} f^{(n)}_{i+1/2} \int_{-h/2}^{h/2} \frac{y^n}{n!}\,dy \\ &= \sum_{n\ \text{even}}^{\infty} f^{(n)}_{i+1/2} \frac{2}{(n+1)!}\left(\frac{h}{2}\right)^{n+1}. \end{aligned} \tag{27.35}$$

It should be noted that, in this exact expression, only the even derivatives of f survive the integration and all derivatives are evaluated at $x_{i+1/2}$. Clearly

other exact expressions are possible, e.g. the integral of $f(x_i + y)$ over the range $0 \le y \le h$, but we will find (27.35) the most useful for our purposes.

Although the preceding discussion has implicitly assumed that both of the limits a and b are finite, with the consequence that N is finite, the general method can be adapted to treat some cases in which one of the limits is infinite. It is sufficient to consider one infinite limit, as an integral with limits $-\infty$ and ∞ can be considered as the sum of two integrals, each with one infinite limit.

Consider the integral

$$I = \int_a^\infty f(x)\,dx,$$

where a is chosen large enough that the integrand is monotonically decreasing for $x > a$ and falls off more quickly than x^{-2}. The change of variable $t = 1/x$ converts this integral into

$$I = \int_0^{1/a} \frac{1}{t^2} f\left(\frac{1}{t}\right) dt.$$

It is now an integral over a finite range and the methods indicated earlier can be applied to it. The value of the integrand at the lower end of the t-range is zero.

In a similar vein, integrals with an upper limit of ∞ and an integrand that is known to behave asymptotically as $g(x)e^{-\alpha x}$, where $g(x)$ is a smooth function, can be converted into an integral over a finite range by setting $x = -\alpha^{-1} \ln \alpha t$. Again, the lower limit, a, for this part of the integral should be positive and chosen beyond the last turning point of $g(x)$. The part of the integral for $x < a$ is treated in the normal way. However, it should be added that if the asymptotic form of the integrand is known to be a linear or quadratic (decreasing) exponential then there are better ways of estimating it numerically; these are discussed in subsection 27.4.3 on Gaussian integration.

We now turn to practical ways of approximating I, given the values of f_i, or a means to calculate them, for $i = 0, 1, \ldots, N$.

27.4.1 Trapezium rule

In this simple case the area shown in figure 27.4(a) is approximated as shown in figure 27.4(b), i.e. by a trapezium. The area A_i of the trapezium is

$$A_i = \tfrac{1}{2}(f_i + f_{i+1})h, \tag{27.36}$$

and if such contributions from all strips are added together then the estimate of the total, and hence of I, is

$$I(\text{estim.}) = \sum_{i=0}^{N-1} A_i = \frac{h}{2}(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{N-1} + f_N). \tag{27.37}$$

This provides a very simple expression for estimating integral (27.34); its accuracy is limited only by the extent to which h can be made very small (and hence N very large) without making the calculation excessively long. Clearly the estimate provided is exact only if $f(x)$ is a linear function of x.

The error made in calculating the area of the strip when the trapezium rule is used may be estimated as follows. The values used are f_i and f_{i+1}, as in (27.36). These can be expressed accurately in terms of $f_{i+1/2}$ and its derivatives by the Taylor series

$$f_{i+1/2\pm1/2} = f_{i+1/2} \pm \frac{h}{2}f'_{i+1/2} + \frac{1}{2!}\left(\frac{h}{2}\right)^2 f''_{i+1/2} \pm \frac{1}{3!}\left(\frac{h}{2}\right)^3 f^{(3)}_{i+1/2} + \cdots .$$

Thus

$$\begin{aligned} A_i(\text{estim.}) &= \tfrac{1}{2}h(f_i + f_{i+1}) \\ &= h\left[f_{i+1/2} + \frac{1}{2!}\left(\frac{h}{2}\right)^2 f''_{i+1/2} + \mathrm{O}(h^4)\right], \end{aligned}$$

whilst, from the first few terms of the exact result (27.35),

$$A_i(\text{exact}) = hf_{i+1/2} + \frac{2}{3!}\left(\frac{h}{2}\right)^3 f''_{i+1/2} + \mathrm{O}(h^5).$$

Thus the error $\Delta A_i = A_i(\text{estim.}) - A_i(\text{exact})$ is given by

$$\begin{aligned} \Delta A_i &= \left(\tfrac{1}{8} - \tfrac{1}{24}\right) h^3 f''_{i+1/2} + \mathrm{O}(h^5) \\ &\approx \tfrac{1}{12}h^3 f''_{i+1/2}. \end{aligned}$$

The total error in $I(\text{estim.})$ is thus given approximately by

$$\Delta I(\text{estim.}) \approx \tfrac{1}{12}nh^3\langle f''\rangle = \tfrac{1}{12}(b-a)h^2\langle f''\rangle, \tag{27.38}$$

where $\langle f''\rangle$ represents an average value for the second derivative of f over the interval a to b.

► *Use the trapezium rule with $h = 0.5$ to evaluate*

$$I = \int_0^2 (x^2 - 3x + 4)\,dx,$$

and, by evaluating the integral exactly, examine how well (27.38) estimates the error.

With $h = 0.5$, we will need five values of $f(x) = x^2 - 3x + 4$ for use in formula (27.37). They are $f(0) = 4$, $f(0.5) = 2.75$, $f(1) = 2$, $f(1.5) = 1.75$ and $f(2) = 2$. Putting these into (27.37) gives

$$I(\text{estim.}) = \frac{0.5}{2}(4 \;+\; 2\times 2.75 \;+\; 2\times 2 \;+\; 2\times 1.75 \;+\; 2) = 4.75.$$

The exact value is

$$I(\text{exact}) = \left[\frac{x^3}{3} - \frac{3x^2}{2} + 4x\right]_0^2 = 4\tfrac{2}{3}.$$