Methods of Theoretical Physics: I

ABSTRACT

First-order and second-order differential equations; Wronskian; series solutions; ordinary and singular points. Orthogonal eigenfunctions and Sturm-Liouville theory. Complex analysis, contour integration. Integral representations for solutions of ODE's. Asymptotic expansions. Methods of stationary phase and steepest descent. Generalised functions.

Books

E.T. Whittaker and G.N. Watson, *A Course of Modern Analysis.*

G. Arfken and H. Weber, *Mathematical Methods for Physicists.*

P.M. Morse and H. Feshbach, *Methods of Theoretical Physics.*

NOTE: These lecture notes are an updated and considerably extended version of the notes previously appearing in two chapters, originally called mch1.ps and mch2.ps on my wesite http://faculty.physics.tamu.edu/pope/mch1.ps and mch2.ps.

(The original mch1.ps and mch2.ps are now at oldmch1.ps and oldmch2.ps.)

Contents

1 First and Second-order Differential Equations

1.1 The Differential Equations of Physics

It is a phenomenological fact that most of the fundamental equations that arise in physics are of second order in derivatives. These may be spatial derivatives, or time derivatives in various circumstances. We call the spatial coordinates and time, the *independent* variables of the differential equation, while the fields whose behaviour is governed by the equation are called the *dependent* variables. Examples of dependent variables are the electromagnetic potentials in Maxwell's equations, or the wave function in quantum mechanics. It is frequently the case that the equations are *linear* in the dependent variables. Consider, for example, the scalar potential ϕ in electrostatics, which satisfies

$$\nabla^2\phi = -4\pi\,\rho \tag{1.1}$$

where ρ is the charge density. The potential ϕ appears only linearly in this equation, which is known as Poisson's equation. In the case where there are no charges present, so that the right-hand side vanishes, we have the special case of Laplace's equation.

Other linear equations are the Helmholtz equation $\nabla^2\psi+k^2\,\psi = 0$, the diffusion equation $\nabla^2\psi - \partial\psi/\partial t = 0$, the wave equation $\nabla^2\psi - c^{-2}\,\partial^2\psi/\partial t^2 = 0$, and the Schrödinger equation $-\hbar^2/(2m)\nabla^2\psi + V\,\psi - \mathrm{i}\hbar\,\partial\psi/\partial t = 0$.

The reason for the linearity of most of the fundamental equations in physics can be traced back to the fact that the fields in the equations do not usually act as sources for *themselves*. Thus, for example, in electromagnetism the electric and magnetic fields respond to the sources that create them, but they do not themselves act as sources; the electromagnetic fields themselves are *uncharged*; it is the electrons and other particles that carry charges that act as the sources, while the photon itself is neutral. There are in fact generalisations of Maxwell's theory, known as Yang-Mills theories, which play a fundamental rôle in the description of the strong and weak nuclear forces, which *are* non-linear. This is precisely because the Yang-Mills fields themselves carry the generalised type of electric charge.

Another fundamental theory that has non-linear equations of motion is gravity, described by Einstein's general theory of relativity. The reason here is very similar; *all* forms of energy (mass) act as sources for the gravitational field. In particular, the energy in the gravitational field itself acts as a source for gravity, hence the non-linearity. Of course in the Newtonian limit the gravitational field is assumed to be very weak, and all the non-linearities disappear.

In fact there is every reason to believe that if one looks in sufficient detail then even the linear Maxwell equations will receive higher-order non-linear modifications. Our best candidate for a unified theory of all the fundamental interactions is string theory, and the way in which Maxwell's equations emerge there is as a sort of "low-energy" effective theory, which will receive higher-order non-linear corrections. However, at low energy scales, these terms will be insignificantly small, and so we won't usually go wrong by assuming that Maxwell's equations are good enough.

The story with the *order* of the fundamental differential equations of physics is rather similar too. Maxwell's equations, the Schrödinger equation, and Einstein's equations are all of second order in derivatives with respect to (at least some of) the independent variables. If you probe more closely in string theory, you find that Maxwell's equations and the Einstein equations will also receive higher-order corrections that involve larger numbers of time and space derivatives, but again, these are insignificant at low energies. So in some sense one should probably ultimately take the view that the fundamental equations of physics tend to be of second order in derivatives because those are the only important terms at the energy scales that we normally probe.

We should certainly expect that at least second derivatives will be observable, since these are needed in order to describe wave-like motion. For Maxwell's theory the existence of wave-like solutions (radio waves, light, *etc.*) is a commonplace observation, and probably in the not too distant future gravitational waves will be observed too.

1.2 First-order Equations

Differential equations involving only one independent variable are called *ordinary* differentials equations, or ODE's, by contrast with *partial* differential equations, or PDE's, which have more than one independent variable. Even first-order ODE's can be complicated.

One situation that is easily solvable is the following. Suppose we have the single first-order ODE

$$\frac{dy}{dx} = F(x)\,. \tag{1.2}$$

The solution is, of course, simply given by $y(x) = \int^x dx' F(x')$ (note that x' here is just a name for the "dummy" integration variable). This is known as "reducing the problem to quadratures," meaning that it now comes down to just performing an indefinite integral. Of course it may or may not be be that the integral can be evaluated explicitly, but that is a different issue; the equation can be regarded as having been solved.

More generally, we could consider a first-order ODE of the form

$$\frac{dy}{dx} = F(x,y)\,. \tag{1.3}$$

A special class of function $F(x,y)$ for which can can again easily solve the equation explicitly is when

$$F(x,y) = -\frac{P(x)}{Q(y)}\,, \tag{1.4}$$

implying that (1.3) becomes $P(x)\,dx + Q(y)\,dy = 0$, since then we can reduce the solution to quadratures, with

$$\int^x dx'\, P(x') + \int^y dy'\, Q(y') = 0\,. \tag{1.5}$$

Note that no assumption of linearity is needed here.

A rather more general situation is when

$$F(x,y) = -\frac{P(x,y)}{Q(x,y)}\,, \tag{1.6}$$

and the differential $P(x,y)\,dx + Q(x,y)\,dy$ is *exact*, which means that we can find a function $\varphi(x,y)$ such that

$$d\varphi(x,y) = P(x,y)\,dx + Q(x,y)\,dy\,. \tag{1.7}$$

Of course there is no guarantee that such a φ will exist. Clearly a *necessary* condition is that

$$\frac{\partial P(x,y)}{\partial y} = \frac{\partial Q(x,y)}{\partial x}\,, \tag{1.8}$$

since $d\varphi = \partial\varphi/\partial x\, dx + \partial\varphi/\partial y\, dy$, which implies we must have

$$\frac{\partial\varphi}{\partial x} = P(x,y)\,, \qquad \frac{\partial\varphi}{\partial y} = Q(x,y)\,, \tag{1.9}$$

since second partial derivatives of φ commute:

$$\frac{\partial^2\varphi}{\partial x\partial y} = \frac{\partial^2\varphi}{\partial y\partial x}\,. \tag{1.10}$$

In fact, one can also see that (1.8) is *sufficient* for the existence of the function φ; the condition (1.8) is known as an *integrability condition* for φ to exist. If φ exists, then solving the differential equation (1.3) reduces to solving $d\varphi = 0$, implying $\varphi(x,y) = c$ =constant. Once $\varphi(x,y)$ is known, this implicitly gives y as a function of x.

If $P(x,y)$ and $Q(x,y)$ do not satisfy (1.8) then all is not lost, because we can recall that solving the differential equation (1.3), where $F(x,y) = -P(x,y)/Q(x,y)$ means solving $P(x,y)\,dx + Q(x,y)\,dy = 0$, which is equivalent to solving

$$\alpha(x,y)\,P(x,y)\,dx + \alpha(x,y)\,Q(x,y)\,dy = 0\,, \tag{1.11}$$

where $\alpha(x,y)$ is some generically non-vanishing but as yet otherwise arbitrary function. If we want the left-hand side of *this* equation to be an exact differential,

$$d\varphi = \alpha(x,y)\,P(x,y)\,dx + \alpha(x,y)\,Q(x,y)\,dy\,, \tag{1.12}$$

then we have the less restrictive integrability condition

$$\frac{\partial(\alpha(x,y)P(x,y))}{\partial y} = \frac{\partial(\alpha(x,y)\,\partial Q(x,y))}{\partial x}\,, \tag{1.13}$$

where we can choose $\alpha(x,y)$ to be more or less anything we like in order to try to ensure that this equation is satisfied. It turns out that some such $\alpha(x,y)$, known as an *integrating factor*, always exists in this case, and so in principle the differential equation is solved. The only snag is that there is no completely systematic way for finding $\alpha(x,y)$, and so one is not necessarily guaranteed actually to be able to determine $\alpha(x,y)$.

1.2.1 Linear first-order ODE

Consider the case where the function $F(x,y)$ appearing in (1.3) is linear in y, of the form $F(x,y) = -p(x)\,y + q(x)$. Then the differential equation becomes

$$\frac{dy}{dx} + p(x)\,y = q(x)\,, \tag{1.14}$$

which is in fact the most general possible form for a first-order linear equation. The equation can straightforwardly be solved explicitly, since now it is rather easy to find the required integrating factor α that renders the left-hand side an exact differential. In particular, α is just a function of x here. Thus we multiply (1.14) by $\alpha(x)$,

$$\alpha(x)\,\frac{dy}{dx} + \alpha(x)\,p(x)\,y = \alpha(x)\,q(x)\,, \tag{1.15}$$

and require $\alpha(x)$ to be such that the left-hand side can be rewritten as

$$\frac{d(\alpha(x)\,y)}{dx} = \alpha(x)\,q(x)\,, \tag{1.16}$$

i.e.

$$\alpha(x)\,\frac{dy}{dx} + \frac{d\alpha(x)}{dx}\,y = \alpha(x)\,q(x)\,. \tag{1.17}$$

Comparing with (1.15), we see that $\alpha(x)$ must be chosen so that

$$\frac{d\alpha(x)}{dx} = \alpha(x)\,p(x)\,, \tag{1.18}$$

implying that we will have

$$\alpha(x) = \exp\Big(\int^x dx'\,p(x')\Big)\,. \tag{1.19}$$

(The arbitrary integration constant just amounts to a constant rescaling of $\alpha(x)$, which obviously is an arbitrariness in our freedom to choose an integrating factor.)

With $\alpha(x)$ in principle determined by the integral (1.19), it is now straightforward to integrate the differential equation written in the form (1.16), giving

$$y(x) = \frac{1}{\alpha(x)} \int^x dx'\, \alpha(x')\, q(x')\,. \tag{1.20}$$

Note that the arbitrariness in the choice of the lower limit of the integral implies that $y(x)$ has an additive part $y_0(x)$ amounting to an arbitrary constant multiple of $1/\alpha(x)$,

$$y_0(x) = C\, \exp\Big(-\int^x dx'\, p(x')\Big)\,. \tag{1.21}$$

This is the general solution of the *homogeneous* differential equation where the "source term" $q(x)$ is taken to be zero. The other part, $y(x) - y_0(x)$ in (1.20) is the *particular integral*, which is a specific solution of the inhomogeneous equation with the source term $q(x)$ included.

2 Separation of Variables in Second-order Linear PDE's

2.1 Separation of variables in Cartesian coordinates

If the equation of motion in a particular problem has sufficient symmetries of the appropriate type, we can sometimes reduce the problem to one involving only ordinary differential equations. A simple example of the type of symmetry that can allow this is the spatial translation symmetry of the Laplace equation $\nabla^2\psi = 0$ or Helmholtz equation $\nabla^2\psi + k^2\,\psi = 0$ written in Cartesian coordinates:

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + k^2\,\psi = 0\,. \tag{2.1}$$

Clearly, this equation retains the same form if we shift x, y and z by constants,

$$x \longrightarrow x + c_1\,, \qquad y \longrightarrow y + c_2\,, \qquad z \longrightarrow z + c_3\,. \tag{2.2}$$

This is not to say that any specific *solution* of the equation will be invariant under (2.2), but it does mean that the solutions must transform in a rather particular way. To be precise, if $\psi(x, y, z)$ is one solution of the differential equation, then $\psi(x + c_1, y + c_2, z + c_3)$ must be another.

As is well known, we can solve (2.1) by looking for solutions of the form $\psi(x, y, z) = X(x)\,Y(y)\,Z(z)$. Substituting into (2.1), and dividing by ψ, gives

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} + k^2 = 0\,. \tag{2.3}$$

The first three terms on the left-hand side could depend only on x, y and z respectively, and so the equation can only be consistent for all (x, y, z) if each term is separately constant,

$$\frac{d^2X}{dx^2} + a_1^2\, X = 0\,, \qquad \frac{d^2Y}{dy^2} + a_2^2\, Y = 0\,, \qquad \frac{d^2Z}{dz^2} + a_3^2\, Z = 0\,, \tag{2.4}$$

where the constants satisfy

$$a_1^2 + a_2^2 + a_3^2 = k^2\,, \tag{2.5}$$

and the solutions are of the form

$$X \sim e^{\mathrm{i}a_1\, x}\,, \qquad Y \sim e^{\mathrm{i}a_2\, y}\,, \qquad Z \sim e^{\mathrm{i}a_3\, z}\,. \tag{2.6}$$

The separation constants a_i can be either real, giving oscillatory solutions in that coordinate direction, or imaginary, giving exponentially growing and decaying solutions, provided that the sum (2.5) is satisfied. It will be the boundary conditions in the specific problem being solved that determine whether a given separation constant a_i should be real or imaginary. The general solution will be an infinite sum over all the basic exponential solutions,

$$\psi(x, y, z) = \sum_{a_1, a_2, a_3} c(a_1, a_2, a_3)\, e^{\mathrm{i}a_1\, x}\, e^{\mathrm{i}a_2\, y}\, e^{\mathrm{i}a_3\, z}\,. \tag{2.7}$$

where the separation constants (a_1, a_2, a_3) can be arbitrary, save only that they must satisfy the constraint (2.5). At this stage the sums in (2.7) are really integrals over the continuous ranges of (a_1, a_2, a_3) that satisfy (2.5). Typically, the boundary conditions will ensure that there is only a discrete infinity of allowed triplets of separation constants, and so the integrals becomes sums. In a well-posed problem, the boundary conditions will also fully determine the values of the constant coefficients $c(a_1, a_2, a_3)$.

Consider, for example, a potential-theory problem in which a hollow cube of side 1 is composed of conducting metal plates, where five of them are held at potential zero, while the sixth is held at a constant potential V. The task is to calculate the electrostatic potential $\psi(x, y, z)$ everywhere inside the cube. Thus we must solve Laplace's equation

$$\nabla^2\, \psi = 0\,, \tag{2.8}$$

subject to the boundary conditions that

$$\psi(0, y, z) = \psi(1, y, z) = \psi(x, 0, z) = \psi(x, 1, z) = \psi(x, y, 0) = 0\,, \qquad \psi(x, y, 1) = V\,. \tag{2.9}$$

(we take the face at $z = 1$ to be at potential V, with the other five faces at zero potential.)

Since we are solving Laplace's equation, $\nabla^2\psi = 0$, the constant k appearing in the Helmholtz example above is zero, and so the constraint (2.5) on the separation constants is just

$$a_1^2 + a_2^2 + a_3^2 = 0 \tag{2.10}$$

here. Clearly to match the boundary condition $\psi(0, y, z) = 0$ in (2.9) at $x = 0$ we must have $X(0) = 0$, which means that the combination of solutions $X(x)$ with positive and negative a_1 must be of the form

$$X(x) \sim e^{\mathrm{i}\, a_1\, x} - e^{-\mathrm{i}\, a_1\, x}\,. \tag{2.11}$$

This gives either the sine function, if a_1 is real, or the hypebolic sinh function, if a_1 is imaginary. But we also have the boundary condtion that $\psi(1, y, z) = 0$, which means that $X(1) = 0$. This determines that a_1 must be real, so that we get oscillatory functions for $X(x)$ that can vanish at $x = 1$ as well as at $x = 0$. Thus we must have

$$X(x) \sim \sin(a_1\, x) \tag{2.12}$$

with $\sin(a_1) = 0$, implying $a_1 = m\,\pi$ where m is an integer, which without loss of generality can be assumed to be greater than zero. Similar arguments apply in the y direction. With a_1 and a_2 determined to be real, (2.5) shows that a_3 must be imaginary. The vanishing of $\psi(x, y, 0)$ implies that our general solution is now established to be

$$\psi(x, y, z) = \sum_{m>0}\sum_{n>0} b_{mn}\, \sin(m\,\pi\, x)\, \sin(n\,\pi\, y)\, \sinh(-\pi\, z\, \sqrt{m^2 + n^2})\,. \tag{2.13}$$

Note that we now indeed have a sum over a discrete infinity of separation constants.

Finally, the boundary condition $\psi(x, y, 1) = V$ on the remaining face at $z = 1$ tells us that

$$V = \sum_{m>0}\sum_{n>0} b_{mn}\, \sin(m\,\pi\, x)\, \sin(n\,\pi\, y)\, \sinh(-\pi\, \sqrt{m^2 + n^2})\,. \tag{2.14}$$

This allows us to determine the constants b_{mn}. We use the orthogonality of the sine functions, which in this case is the statement that if m and p are integers we must have

$$\int_0^1 dx\, \sin(m\,\pi\, x)\, \sin(p\,\pi\, x) = 0 \tag{2.15}$$

if p and m are unequal, and

$$\int_0^1 dx\, \sin(m\,\pi\, x)\, \sin(p\,\pi\, x) = \tfrac{1}{2} \tag{2.16}$$

if p and m are equal.[1] This allows us to pick out the term $m = p$, $n = q$ in the double summation (2.14), by multiplying by $\sin(p\,\pi\,x)\,\sin(q\,\pi\,y)$ and integrating over x and y:

$$V \int_0^1 dx \int_0^1 dy\, \sin(p\,\pi\,x)\, \sin(q\,\pi\,y) = \tfrac{1}{4} b_{pq}\, \sinh(-\pi\,\sqrt{p^2+q^2})\,. \tag{2.17}$$

Since $\int_0^1 dx\, \sin(p\,\pi\,x) = [1-(-1)^p]/(p\,\pi)$ we therefore find that b_{pq} is nonzero only when p and q are odd, and then

$$b_{2r+1,2s+1} = \frac{16V}{(2r+1)\,(2s+1)\,\pi^2\, \sinh(-\pi\,\sqrt{(2r+1)^2+(2s+1)^2})} \tag{2.18}$$

All the constants in the original general solution of Laplace's equation have now been determined, and the problem is solved.

2.2 Separation of variables in spherical polar coordinates

Another common example of separability arises when solving the Laplace or Helmholtz equation in spherical polar coordinates (r, θ, ϕ). These are related to the Cartesian coorindates (x, y, z) in the standard way:

$$x = r\,\sin\theta\,\cos\phi\,, \qquad y = r\,\sin\theta\,\sin\phi\,, \qquad z = r\,\cos\theta\,. \tag{2.19}$$

In terms of these, (2.1) becomes

$$\frac{1}{r^2}\,\frac{\partial}{\partial r}\Big(r^2\,\frac{\partial\psi}{\partial r}\Big) + \frac{1}{r^2}\,\nabla^2_{(\theta,\phi)}\,\psi + k^2\,\psi = 0\,, \tag{2.20}$$

where $\nabla^2_{(\theta,\phi)}$ is the two-dimensional Laplace operator on the surface of the unit-radius sphere,

$$\nabla^2_{(\theta,\phi)} \equiv \frac{1}{\sin\theta}\,\frac{\partial}{\partial\theta}\Big(\sin\theta\,\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\,\frac{\partial^2}{\partial\phi^2}\,. \tag{2.21}$$

The Helmholtz equation in spherical polar coordinates can be separated by first writing $\psi(r, \theta, \phi)$ in the form

$$\psi(r,\theta,\phi) = \frac{1}{r}\,R(r)\,Y(\theta,\phi)\,. \tag{2.22}$$

Substituting into the Helmholtz equation (2.20), and dividing out by ψ in the usual way, we get

$$\frac{r^2}{R}\,\frac{d^2R}{dr^2} + \frac{1}{Y}\,\nabla^2_{(\theta,\phi)}Y + r^2\,k^2 = 0\,. \tag{2.23}$$

(It is useful to note that $r^{-2}\partial(r^2\partial\psi/\partial r)/\partial r$ is the same thing as $r^{-1}\partial^2(r\,\psi)/\partial r^2$ when doing this calculation.)

[1] Just use the rules for multiplying products of sine functions to show this. What we are doing here is constructing a Fourier series expansion for the function V, which happens to be taken to be a constant in our example.

The middle term in (2.23) can depend only on θ and ϕ, while the first and third can depend only on r, and so consistency for all (r,θ,ϕ) therefore means that the middle term must be constant, and so

$$\nabla^2_{(\theta,\phi)}\, Y = -\lambda\, Y\,, \qquad \frac{d^2 R}{dr^2} = \Big(\frac{\lambda}{r^2} - k^2\Big)\, R\,. \tag{2.24}$$

The key point now is that one can show that the harmonics $Y(\theta,\phi)$ on the sphere are well-behaved only if the separation constant λ takes a certain discrete infinity of non-negative values. The most elegant way to show this is by making use of the symmetry properties of the sphere, but since this takes us away from the main goals of the course, we will not follow that approach here.[2] Instead, we shall follow the more "traditional," if more pedestrian, approach of examining the conditions under which singular behaviour of the eigenfunction solutions of the differential equation can be avoided.

To study the eigenvalue problem $\nabla^2_{(\theta,\phi)}\, Y = -\lambda\, Y$ in detail, we make a further separation of variables by taking $Y(\theta,\phi)$ to be of the form $Y(\theta,\phi) \sim \Theta(\theta)\,\Phi(\phi)$. Substituting this in, and multiplying by $\sin^2\theta\, Y^{-1}$, we get

$$\frac{1}{\Theta}\,\sin\theta\,\frac{d}{d\theta}\Big(\sin\theta\,\frac{d\Theta}{d\theta}\Big) + \frac{1}{\Phi}\,\frac{d^2\Phi}{d\phi^2} + \lambda\,\sin^2\theta = 0\,. \tag{2.25}$$

By now-familiar arguments the middle term can depend only on ϕ, while the first and last depend only on θ. Consistency for all θ and ϕ therefore implies that the middle term must be a constant, and so we have

$$\frac{d^2\Phi}{d\phi^2} + m^2\,\Phi = 0\,, \tag{2.26}$$

$$\sin\theta\,\frac{d}{d\theta}\Big(\sin\theta\,\frac{d\Theta}{d\theta}\Big) + (\lambda\,\sin^2\theta - m^2)\,\Theta = 0\,. \tag{2.27}$$

[2] The essential point is that the surface of the unit sphere can be defined as $x^2+y^2+z^2=1$, and this is invariant under transformations of the form

$$\begin{pmatrix} x\\ y\\ z\end{pmatrix} \longrightarrow M\,\begin{pmatrix} x\\ y\\ z\end{pmatrix}\,,$$

where M is any constant 3×3 orthogonal matrix, satisfying $M^T\, M = 1\!\!1$. This shows that the sphere is invariant under the 3-parameter group $O(3)$, and hence the eigenfunctions Y must fall into representations under $O(3)$. The calculation of the allowed values for λ, and the forms of the associated eigenfunctions Y, then follow from group-theoretic considerations. Anticipating the result that we shall see by other means, the eigenvalues λ take the form $\lambda_\ell = \ell(\ell+1)$, where ℓ is any non-negative integer. The eigenfunctions are classified by ℓ and a second integer m, with $-\ell \le m \le \ell$, and are the well-known spherical harmonics $Y_{\ell m}(\theta,\phi)$. The fact that λ depends on ℓ but not m means that the eigenvalue $\lambda_\ell = \ell(\ell+1)$ has a degeneracy $(2\ell+1)$.

The solution to the Φ equation is $\Phi \sim e^{\pm \mathrm{i}\, m\, \phi}$. The constant m^2 could, *a priori*, be positive or negative, but we must recall that the coordinate ϕ is periodic on the sphere, with period 2π. The periodicity implies that the eigenfunctions Φ should be periodic too, and hence it must be that m^2 is non-negative. In order that we have $\Phi(\phi + 2\pi) = \Phi(\phi)$ it must furthermore be the case that m is an integer.

To analyse the eigenvalue equation (2.27) for Θ, it is advantageous to define a new independent variable x, related to θ by $x = \cos\theta$. At the same time, let us now use y instead of Θ as our symbol for the dependent variable. Equation (2.27) therefor becomes

$$\frac{d}{dx}\Big((1-x^2)\,\frac{dy}{dx}\Big) + \Big(\lambda - \frac{m^2}{1-x^2}\Big)\, y = 0\,. \tag{2.28}$$

This equation is called the *Associated Legendre Equation*, and it will become necessary to study its properties, and solutions, in some detail in order to be able to construct solutions of the Laplace or Helmholtz equation in spherical polar coordinates. We shall do this in section 3 below. In fact, as we shall see, it is convenient first to study the simpler equation when $m = 0$, which corresponds to the case where the harmonics $Y(\theta, \phi)$ on the sphere are independent of the azimuthal angle ϕ. The equation (2.28) in the case $m = 0$ is called the *Legendre Equation*.

2.3 Separation of variables in cylindrical polar coordinates

Another important second-order equation that can arise from the separation of variables is Bessel's equation, Suppose we are solving Laplace's equation in cylindrical polar coordinates (ρ, ϕ, z), so that we have

$$\frac{1}{\rho}\,\frac{\partial}{\partial\rho}\Big(\rho\frac{\partial\psi}{\partial\rho}\Big) + \frac{1}{\rho^2}\,\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2} = 0\,. \tag{2.29}$$

We can separate variables by writing $\psi(\rho,\phi,z) = R(\rho)\,\Phi(\phi)\,Z(z)$, which leads, after dividing out by ψ, to

$$\frac{1}{\rho\, R}\,\frac{d}{d\rho}\Big(\rho\frac{dR}{d\rho}\Big) + \frac{1}{\rho^2\,\Phi}\,\frac{d^2\Phi}{d\phi^2} + \frac{1}{Z}\,\frac{d^2 Z}{dz^2} = 0\,. \tag{2.30}$$

We can therefore deduce that

$$\frac{d^2 Z}{dz^2} - k^2\, Z = 0\,, \qquad \frac{d^2\Phi}{d\phi^2} + \nu^2\,\Phi = 0\,, \tag{2.31}$$

$$\frac{d^2 R}{d\rho^2} + \frac{1}{\rho}\,\frac{dR}{d\rho} + \Big(k^2 - \frac{\nu^2}{\rho^2}\Big)\, R = 0\,, \tag{2.32}$$

where k^2 and ν^2 are separation constants. Rescaling the radial coordinate by defining $x = k\,\rho$, and renaming R as y, the last equation takes the form

$$x^2\,\frac{d^2y}{dx^2} + x\,\frac{dy}{dx} + (x^2 - \nu^2)\, y = 0\,. \tag{2.33}$$

This is Bessel's equation; we shall return later to a study of its solutions.

3 Solutions of the Associated Legendre Equation

We shall now turn to a detailed study of the solutions of the associated Legendre equation, which we obtained in our separation of variables in spherical polar coordinates in section 2.2.

3.1 Series solution of the Legendre equation

We begin by considering the simpler case where the separation constant m is zero, implying that the associated Legendre equation (2.28) reduces to the Legendre equation

$$[(1-x^2)\, y']' + \lambda\, y = 0\,. \tag{3.1}$$

Note that here we are denoting a derivative with respect to x by a prime, so that dy/dx is written as y', and so on. We shall use (3.1) to introduce the method of solution of linear ODE's by series solution, known sometimes as the *Frobenius Method*.

The idea essentially is to develop a solution as a power series in the independent variable x, with expansion coefficients determined by substituting the series into the differential equation, and equating terms order by order in x. The method is of wide applicability; here we shall take the Legendre equation as an example to illustrate the procedure.

We begin by writing the series expansion

$$y = \sum_{n\ge 0} a_n\, x^n\,. \tag{3.2}$$

(In more general circumstances, which we shall study later, we shall need to consider series expansions of the form $y(x) = \sum_{(n)\ge 0} a_n\, x^{n+\sigma}$, where σ may not necessarily be an integer. But in the present case, for reasons we shall see later, we do not need the x^σ factor at all.) Clearly we shall have

$$y' = \sum_{n\ge 0} n\, a_n\, x^{n-1}\,, \qquad y'' = \sum_{n\ge 0} n\,(n-1)\, a_n\, x^{n-2}\,. \tag{3.3}$$

Substituting into equation (3.1), we find

$$\sum_{n\ge 0} n\,(n-1)\, a_n\, x^{n-2} + \sum_{n\ge 0} (\lambda - n\,(n+1))\, a_n\, x^n = 0\,. \tag{3.4}$$

Since we want to equate terms order by order in x, it is useful to shift the summation variable by 2 in the first term, by writing $n = m + 2$;

$$\sum_{n\ge 0} n\,(n-1)\,a_n\,x^{n-2} = \sum_{m\ge -2} (m+2)(m+1)\,a_{m+2}\,x^m = \sum_{m\ge 0} (m+2)(m+1)\,a_{m+2}\,x^m\,. \tag{3.5}$$

(The last step, where we have dropped the $m = -2$ and $m = -1$ terms in the summation, clearly follows from the fact that the $(m+2)(m+1)$ factor gives zero for these two values of m.) Finally, relabelling m as n again, we get from (3.4)

$$\sum_{n\ge 0} \Big((n+2)(n+1)\,a_{n+2} + (\lambda - n\,(n+1))\,a_n\Big)\,x^n = 0\,. \tag{3.6}$$

Since this must hold for all values of x, it follows that the coefficient of each power of x must vanish separately, giving

$$(n+2)(n+1)\,a_{n+2} + (\lambda - n\,(n+1))\,a_n = 0 \tag{3.7}$$

for all $n \ge 0$. Thus we have the recursion relation

$$a_{n+2} = \frac{n\,(n+1) - \lambda}{(n+1)(n+2)}\,a_n\,. \tag{3.8}$$

We see from (3.8) that all the coefficients a_n with $n \ge 2$ can be solved for, in terms of a_0 and a_1. In fact all the a_n for *even* n can be solved for in terms of a_0, while all the a_n for *odd* n can be solved for in terms of a_1. Since the equation is linear, we can take the even-n series and the odd-n series as the two independent solutions of the Legendre equation, which we can call $y_1(x)$ and $y_2(x)$:

$$\begin{aligned} y_{(1)}(x) &= a_0 + a_2\,x^2 + a_4\,x^4 + \cdots\,, \\ y_{(2)}(x) &= a_1 + a_3\,x^3 + a_5\,x^5 + \cdots\,. \end{aligned} \tag{3.9}$$

The first solution involves only the even a_n, and thus has only even powers of x, whilst the second involves only the odd a_n, and has only odd powers of x. We can conveniently consider the two solutions separately, by taking either $a_1 = 0$, to discuss $y_{(1)}$, or else taking $a_0 = 0$, to discuss $y_{(2)}$.

Starting with y_1, we therefore have from (3.8) that $a_2 = -\frac{1}{2}\lambda\,a_0$, $a_3 = 0$, $a_4 = \frac{1}{12}(6 - \lambda)\,a_2$, $a_5 = 0$, *etc.*. In the expression for a_4, we can substitute the expression already found for a_2, and so on. Thus we will get

$$\begin{aligned} a_2 &= -\tfrac{1}{2}\lambda\,a_0\,, \qquad a_4 = -\tfrac{1}{12}\lambda\,(6-\lambda)\,a_0\,, \qquad \ldots \\ a_3 &= a_5 = a_7 = \cdots = 0\,. \end{aligned} \tag{3.10}$$

The series solution in this case is therefore given by

$$y_{(1)} = a_0 \Big(1 - \tfrac{1}{2}\lambda\, x^2 - \tfrac{1}{12}\lambda\,(6-\lambda)\, x^4 + \cdots\Big)\,. \tag{3.11}$$

To discuss the solution $y_{(2)}$ instead, we can take $a_0 = 0$ and $a_1 \ne 0$. The recursion relation (3.8) now gives $a_2 = 0$, $a_3 = \frac{1}{6}(2-\lambda)\, a_1$, $a_4 = 0$, $a_5 = \frac{1}{20}(12-\lambda)\, a_3$, $a_5 = 0$, *etc.*, and so we find

$$\begin{aligned} a_3 &= \tfrac{1}{6}(2-\lambda)\, a_1\,, \qquad a_5 = \tfrac{1}{120}(2-\lambda)\,(12-\lambda)\, a_1\,, \qquad \ldots \\ a_2 &= a_4 = a_6 = \cdots = 0\,. \end{aligned} \tag{3.12}$$

The series solution in this case therefore has the form

$$y_{(2)} = a_1 \Big(x + \tfrac{1}{6}(2-\lambda)\, x^3 + \tfrac{1}{120}(2-\lambda)\,(12-\lambda)\, x^5 + \cdots\Big)\,. \tag{3.13}$$

To summarise, we have produced two independent solutions to our differential equation (3.1), which are given by (3.11) and (3.13). The fact that they are independent is obvious, since the first is an even function of x whilst the second is an odd function. To make this precise, we should say that $y_{(1)}(x)$ and $y_{(2)}(x)$ are *linearly-independent*, meaning that the only possible solution for constants α and β in the equation

$$\alpha\, y_{(1)}(x) + \beta\, y_{(2)}(x) = 0 \tag{3.14}$$

is $\alpha = 0$ and $\beta = 0$. In other words, $y_{(1)}(x)$ and $y_{(2)}(x)$ are not related by any constant factor of proportionality. We shall show later that any second-order ordinary differential equation must have exactly two linearly-independent solutions, and so with our solutions $y_{(1)}(x)$ and $y_{(2)}(x)$ established to be linearly-independent, this means that we have obtained the most general possible solution to (3.1).

The next question is what can we do with our series solutions (3.11) and (3.13). They are, in general, infinite series. Whenever one encounters an infinite series, one needs to worry about whether the series converges to a finite result. For example, the series

$$S_1 \equiv \sum_{n\ge 0} 2^{-n} = 1 + \tfrac{1}{2} + \tfrac{1}{4} + \tfrac{1}{8} + \tfrac{1}{16} + \cdots \tag{3.15}$$

converges, giving $S_1 = 2$, whilst the series

$$S_2 \equiv \sum_{n\ge 0} 2^{n} = 1 + 2 + 4 + 8 + 16 + \cdots \tag{3.16}$$

diverges, giving $S_2 = \infty$. Another series that diverges is

$$S_3 = \sum_{n\ge 0} \frac{1}{n+1} = 1 + \tfrac{1}{2} + \tfrac{1}{3} + \tfrac{1}{4} + \tfrac{1}{5} + \cdots\,. \tag{3.17}$$

For our solutions (3.11) and (3.13), we must find out for what range of values of x do the series converge.

One way to test the converge of a series is by applying the *ratio test.* This test says that the series $f = \sum_{n\ge 0} w_n$ converges if the ratio $R_n \equiv w_{n+1}/w_n$ is less than 1 in the limit $n \longrightarrow \infty$. The series converges if $R_\infty < 1$, it diverges if $R_\infty > 1$, and one gains no information in the marginal case where $R_\infty = 1$. We won't prove the ratio test here, but it is clearly plausible. It essentially says that if each successive term in the series (at least when we go a long way down the series) is smaller than its predecessor by some fraction less than 1, then the sum of all the terms is finite. If on the other hand each successive term is bigger than its predecessor by some factor greater than 1, then the sum of all the terms will be infinite. We can try out the ratio test on the three examples in (3.15), (3.16) and (3.17). Sure enough, for the convergent series (3.15) we find the ratio of the $(n+1)$'th term to the n'th term is

$$R_n \equiv \frac{1/2^{n+1}}{1/2^n} = \tfrac{1}{2} \tag{3.18}$$

and so this has the limit $R_\infty = \frac{1}{2}$ which is less than 1. For the second example (3.16) we have $R_n = 2$, and so $R_\infty = 2$. The ratio test therefore predicts that this series will diverge. For the third example, we see from (3.17) that

$$R_n = \frac{n+1}{n+2}\,, \tag{3.19}$$

and so $R_\infty = 1$. The ratio test doesn't give us any result in this case therefore. However, a more involved calculation will show that the series (3.17) diverges.

Going back to our series solutions (3.2), we have

$$R_n = \frac{a_{n+2}\, x^{n+2}}{a_n\, x^n} = \frac{a_{n+2}}{a_n}\, x^2\,, \tag{3.20}$$

From (3.8), this can be written as

$$R_n = \frac{n\,(n+1) - \lambda}{(n+1)\,(n+2)}\, x^2\,. \tag{3.21}$$

For sufficiently large n we can neglect the contribution from the fixed given value of λ, and so the terms proportional to n^2 in the numerator and denominator dominate at large n. Thus we have

$$R_\infty = x^2\,. \tag{3.22}$$

Recall that in our problem, $x = \cos\theta$, and so we are interested in x in the range $-1 \le x \le 1$. If $|x| < 1$, the ratio test tells us that the series converges. However, we would also like to know what happens at $x = \pm 1$, since these points correspond to $\theta = 0$ and $\theta = \pi$, the north and south poles of the sphere. Here, the ratio test fails to give us any information, although it does tell us that the series diverges for $|x| > 1$.

A more sophisticated analysis shows that the series will in fact always diverge at $x = \pm 1$, unless λ takes a value such that the series terminates. Obviously, if the series terminates after a finite number of terms, then there can be no possibility of the sum diverging. For the termination to occur, the numerator in (3.8) must vanish for some value of n. Clearly, a necessary condition for this to occur is that ℓ must be a positive integer of the form $n\,(n+1)$. In fact the even series for $y_1(x)$ terminates if $\lambda = \ell(\ell+1)$, where ℓ is an even non-negative integer, whilst the odd series for $y_{(2)}$ terminates if ℓ is an odd positive integer. Once a_n becomes zero for some value of n, it is obvious from the recursion relation (3.8) that all the higher coefficients $a_{n+2}, a_{n+4}, \ldots$ will vanish too.

As an example to illustrate the divergent behaviour if the series does not terminate, consider the odd series $y_2(x)$, with $\lambda = 0$. From (3.8) we then have $a_{n+2} = n\,a_n/(n+2)$ (with n odd), which has the solution $a_n = a_1/n$. Thus the series (3.2) becomes

$$y = a_0\,(x + \tfrac{1}{3}x^3 + \tfrac{1}{5}x^5 + \tfrac{1}{7}x^7 + \cdots)\,, \qquad (3.23)$$

which can be recognised as the power-series expansion of

$$y = \tfrac{1}{2}a_1\,\log\Big(\frac{1+x}{1-x}\Big)\,, \qquad (3.24)$$

which clearly diverges at $x = \pm 1$. For all other values of λ that lead to non-terminating series, one similarly finds a logarithmic divergence at $x = \pm 1$.

To recapitulate, we have seen that if we want the solutions of the Legendre equation to be well-behaved at $x = \pm 1$, which we usually do since we wish to obtain solutions of the original Laplace or Helmholtz equation that are well-behaved on the sphere, then only those solutions for which the series (3.2) terminates are acceptable. This occurs when the eigenvalue λ in (3.1) takes the form

$$\lambda = \ell(\ell+1)\,, \qquad (3.25)$$

where ℓ is a non-negative integer, with the corresponding eigenfunctions y being polynomials in x of degree ℓ. Note that if ℓ is even, the polynomial will involve only even powers of x, while if ℓ is odd, the polynomial will involve only odd powers of x. It is easy to work out the first few examples, by using (3.8) to solve recursively for the expansion coefficients in (3.2). By convention the ℓ'th Legendre polynomial is denoted by $P_\ell(x)$, and is normalised so that $P_\ell(1) = 1$. The first few are therefore given by

$$\begin{aligned} &P_0(x) = 1\,, \qquad P_1(x) = x\,, \qquad P_2(x) = \tfrac{1}{2}(3x^2 - 1)\,, \\ &P_3(x) = \tfrac{1}{2}(5x^3 - 3x)\,, \qquad P_4(x) = \tfrac{1}{8}(35x^4 - 30x^2 + 3)\,. \end{aligned} \tag{3.26}$$

A similar analysis for the case where m is non-zero shows that the associated Legendre equation (2.28) has solutions regular at $x = \pm 1$ only if ℓ is a non-negative integer, and m is an integer taking any of the values in the range $-\ell \le m \le \ell$. The corresponding eigenfunctions are the associated Legendre functions $P_\ell^m(x)$. It can be shown that these are related to the Legendre polynomials $P_\ell(x)$ by the formula

$$P_\ell^m(x) = (-1)^m\,(1-x^2)^{m/2}\,\frac{d^m P_\ell(x)}{dx^m}\,. \tag{3.27}$$

We shall return to these later.

3.2 Properties of the Legendre polynomials

The Legendre polynomials $P_\ell(x)$ are the basic set of regular solutions of the Legendre equation,

$$\frac{d}{dx}\Big((1-x^2)\,\frac{dP_\ell(x)}{dx}\Big) + \ell\,(\ell+1)\,P_\ell(x) = 0\,, \tag{3.28}$$

and this is the equation that arose (in the azimuthally-symmetric case) when separating variables in spherical polar coordinates. It follows that in order to construct solutions of the Laplace equation by the method of separating the variables, we shall therefore need to have a thorough understanding of the properties of the Legendre polynomials.

The basic technique that one uses for solving an equation such as the Laplace equation in spherical polar coordinates is parallel to that which we used in section (2.1) when we discussed the analogous problem in Cartesian coordinates. Namely, we write down the most general possible solution (obtained by separation of variables), and then determine the constant coefficients in the expansion by matching to given boundary data. As we shall see below, this means in particular that we need to be able to determine the coefficients a_ℓ in the expansion of an arbitrary function $f(x)$ in terms of Legendre polynomials;

$$f(x) = \sum_{\ell \ge 0} a_\ell\,P_\ell(x)\,. \tag{3.29}$$

For now we shall just assume that such an expansion is possible; the proof is a little involved, and we shall postpone this until a bit later in the course, where we shall prove it in a much more general context.[3]

[3] The series (3.29) is a generalisation of the familiar Fourier series.

The essential requirement in order to be able to determine the constants a_ℓ is to know some appropriate *orthogonality relation* among the Legendre polynomials. Specifically, we can show that

$$\int_{-1}^{1} dx\, P_\ell(x)\, P_n(x) = 0\,, \qquad \ell \neq n\,, \tag{3.30}$$

and

$$\int_{-1}^{1} dx\, P_\ell(x)\, P_n(x) = C_n\,, \qquad \ell = n\,. \tag{3.31}$$

The constants C_n are calculable (once one has defined a normalisation for the Legendre polynomials), and we shall calculate them, and prove the orthogonality condition (3.30) below. It is clear that with these results we can then calculate the coefficients a_ℓ in the series expansion (3.29). We just multiply (3.29) by $P_n(x)$ and integrate over x, to get

$$\begin{aligned}\int_{-1}^{1} dx\, P_n(x)\, f(x) &= \sum_{\ell\ge 0} a_\ell \int_{-1}^{1} dx\, P_\ell(x)\, P_n(x)\,,\\ &= a_n\, C_n\,. \end{aligned}\tag{3.32}$$

Hence we solve for the coefficients a_n, giving

$$a_n = \frac{1}{C_n}\int_{-1}^{1} dx\, P_n(x)\, f(x)\,. \tag{3.33}$$

The proof of orthogonality of the Legendre polynomials, as in (3.30), is very simple. We take the Legendre equation (3.28) and multiply it by $P_n(x)$, and then subtract from this the same thing with the roles of ℓ and n exchanged:

$$[(1-x^2)\, P_\ell']'\, P_n - [(1-x^2)\, P_n']'\, P_\ell + [\ell\,(\ell+1) - n\,(n+1)]\, P_\ell\, P_n = 0\,. \tag{3.34}$$

(It is understood that P_ℓ and P_n here are functions of x, and that a prime means d/dx.) We now integrate over x, from $x=-1$ to $x=+1$, and note that using an integration by parts we shall have

$$\int_{-1}^{1} dx\, [(1-x^2)\, P_\ell']'\, P_n = -\int_{-1}^{1} dx\, [(1-x^2)\, P_\ell'\, P_n' + \Big[(1-x^2)\, P_\ell'(x)\, P_n(x)\Big]_{-1}^{1}\,. \tag{3.35}$$

The boundary terms here at $x=\pm 1$ vanish, because of the $(1-x^2)$ factor. Thus after integrating (3.34) and integrating by parts on the first two terms, we get simply

$$[\ell\,(\ell+1) - n\,(n+1)] \int_{-1}^{1} dx\, P_\ell(x)\, P_n(x) = 0\,. \tag{3.36}$$

This means that either $\ell\,(\ell+1)$ equals $n\,(n+1)$, or else

$$\int_{-1}^{1} dx\, P_\ell(x)\, P_n(x) = 0\,, \qquad \ell \neq n\,. \tag{3.37}$$

Since it is always understood that ℓ and n are non-negative integers, we see that $\ell\,(\ell+1)$ is equal to $n\,(n+1)$ only if $\ell = n$. Thus if have proved the orthogonality of the Legendre polynomials; if ℓ and n are not equal, then (3.37) is satisfied.

The next step takes a little more work. We need to calculate the constants C_n occurring in the integral (3.31). Of course we can only do that once we have decided upon a normalisation for the Legendre polynomials $P_\ell(x)$. By convention, they are defined to be such that

$$P_\ell(1) = 1\,. \tag{3.38}$$

In order to evaluate the integral in (3.31), we now need to have an explicit way of expressing the Legendre polynomials. It turns out that a convenient way to do this is in terms of a representation called *Rodrigues' Formula*. This formula asserts that $P_\ell(x)$, with the normalisation (3.38), can be written as

$$P_\ell(x) = \frac{1}{2^\ell\,\ell!}\,\frac{d^\ell}{dx^\ell}\,(x^2-1)^\ell\,. \tag{3.39}$$

We can prove Rodrigues' formula in two stages. First, we shall prove that it gives some constant multiple of $P_\ell(x)$. Then, we shall prove that in fact from the definition (3.39), we shall have $P_\ell(1) = 1$. To prove the first stage, let's get rid of the superfluous baggage of messy constant factors, and consider

$$f_\ell(x) \equiv \frac{d^\ell}{dx^\ell}\,(1-x^2)^\ell\,. \tag{3.40}$$

The technique now will be to show that $f_\ell(x)$ satisfies the Legendre equation (3.28), and hence, since $f_\ell(x)$ is manifestly just a *polynomial* function of x, it *must* therefore be some constant multiple of the Legendre polynomial $P_\ell(x)$.

Using the binomial theorem,

$$(1+z)^\ell = \sum_{k=0}^{\ell} \begin{pmatrix} \ell \\ k \end{pmatrix} z^k\,, \qquad \text{where} \qquad \begin{pmatrix} \ell \\ k \end{pmatrix} \equiv \frac{\ell!}{k!\,(\ell-k)!}\,, \tag{3.41}$$

where we shall take $z = -x^2$, we get

$$f_\ell(x) = \frac{d^\ell}{dx^\ell} \sum_{k=0}^{\ell} (-1)^k \begin{pmatrix} \ell \\ k \end{pmatrix} x^{2k}\,. \tag{3.42}$$

Using the fact that

$$\frac{d^\ell}{dx^\ell}\,x^{2k} = 2k\,(2k-1)\cdots(2k-\ell+1)\,x^{2k-\ell} = \frac{(2k)!}{(2k-\ell)!}\,x^{2k-\ell}\,, \tag{3.43}$$

we therefore obtain the series expansion

$$f_\ell(x) = \sum_{k=0}^{\ell} (-1)^k \begin{pmatrix} \ell \\ k \end{pmatrix} \frac{(2k)!}{(2k-\ell)!}\, x^{2k-\ell}\,. \tag{3.44}$$

What we have obtained here is a polynomial series in x. Now we have already studied the series expansion for solutions of the Legendre equation; we wrote them as (3.2), and we showed that the expansion coefficients a_n must satisfy (3.8). All we have to do in order to prove that our function $f_\ell(x)$ satisfies the Legendre equation is to show that the coefficients of the powers of x in (3.44) satisfy the same recursion relation (3.8).

We can express (3.44) as a series $f_\ell = \sum_{n=0}^{\ell} a_n\, x^n$. Comparing coefficients, we see that $2k - \ell = n$ and hence $k = (n+\ell)/2$. Thus we can read off the coefficients

$$a_n = \frac{(-1)^{\frac12(n+\ell)}\, \ell!\, (n+\ell)!}{n!\, \Big(\frac12(\ell+n)\Big)!\, \Big(\frac12(\ell-n)\Big)!}\,. \tag{3.45}$$

Using $(p+1)! = (p+1)\, p!$ in the various terms, it is now easy to see that if we use (3.45) to calculate a_{n+2}, we can write it as

$$a_{n+2} = \frac{(n-\ell)(n+\ell+1)}{(n+1)(n+2)}\, a_n\,. \tag{3.46}$$

This is exactly the same as the recursion relation (3.8), and so this proves that the functions $f_\ell(x)$ defined in (3.40) satisfy the Legendre equation with $\lambda = \ell\,(\ell+1)$. (Check for yourself that this is a correct statement both for ℓ even and ℓ odd.) Since $P_\ell(x)$ given in Rodrigues' formula (3.39) is just a constant multiple of $f_\ell(x)$, i.e.

$$P_\ell(x) = \frac{(-1)^\ell}{2^\ell\, \ell!}\, f_\ell(x)\,, \tag{3.47}$$

it follows that we have established the first part of our proof; up to constant normalisation, we have verified that the Rodrigues' formula (3.39) does indeed give polynomial solutions of the Legendre equation (3.28), and so it must be that

$$P_\ell(x) = c\, f_\ell(x)\,, \tag{3.48}$$

where c is some constant of proportionality.

Determining c is easily done, by noting that we can write (3.40) as

$$f_\ell(x) = \frac{d^\ell}{dx^\ell}\, [(1-x)^\ell\, (1+x)^\ell]\,. \tag{3.49}$$

We want to calculate $f_\ell(1)$, since c will be determined from $1 = P_\ell(1) = c\, f_\ell(1)$. Looking at (3.49), it is evident that when we distribute the ℓ derivatives over the factors in the square brackets, any term where a factor of $(1-x)$ survives will give zero when we set $x=1$. The only term that will survive upon setting $x=1$ is therefore the term where all ℓ of the derivatives land on $(1-x)^\ell$. This gives

$$\frac{d^\ell}{x^\ell}\,(1-x)^\ell = (-1)^\ell\,\ell!\,. \tag{3.50}$$

Setting $x=1$ in the $1+x)^\ell$ factor (which will be left undifferentiated since all the derivatives had to land on $(1-x)^\ell$) gives a 2^ℓ. Thus we have $f_\ell(1) = (-1)^\ell\,\ell!\,2^\ell$, and so from (3.48) we find $c = (-1)^\ell\,/(\ell!\,2^\ell)$, and hence

$$P_\ell(x) = \frac{1}{2^\ell\,\ell!}\,\frac{d^\ell}{dx^\ell}\,(x^2-1)^\ell\,. \tag{3.51}$$

This completes the proof of Rodrigues' Formula for the Legendre polynomials.

Lest our original task has been forgotten during the course of this discussion, let us remind ourselves that we wanted to determine the constants C_n in (3.31). That is, we want to calculate

$$C_n = \int_{-1}^1 dx\,[P_n(x)]^2\,. \tag{3.52}$$

From Rodrigues' formula (3.39), we can write this as

$$C_n = \frac{1}{2^{2n}\,(n!)^2}\,\int_{-1}^1 dx\,\partial^n(x^2-1)^n\,\partial^n(x^2-1)^n\,, \tag{3.53}$$

where we write ∂^n instead of d^n/dx^n for brevity. Integrating by parts n times, and noting that the powers of (x^2-1) will kill off the resulting boundary terms, we therefore have

$$C_n = \frac{(-1)^n}{2^{2n}\,(n!)^2}\,\int_{-1}^1 dx\,(x^2-1)^n\,\partial^{2n}(x^2-1)^n\,. \tag{3.54}$$

Now $(x^2-1)^{(n)}$ is a polynomial in x, which looks like $x^{2n}+\cdots$, where the ellipses denote terms of lower order in x. When we differentiate $2n$ times, only the first term gives a contribution, and so from $\partial^{2n}\,x^{2n} = (2n)!$ we find that

$$C_n = \frac{(2n)!}{2^{2n}\,(n!)^2}\,\int_{-1}^1 dx\,(1-x^2)^n\ . \tag{3.55}$$

Unfortunately our troubles are not yet quite over, because the integral is not going to give up without a bit of a fight. The best way to evaluate it is by induction. We note that we can write the following:

$$(1-x^2)^n = (1-x^2)(1-x^2)^{n-1} = (1-x^2)^{n-1} + \frac{x}{2n}\,\frac{d}{dx}\,(1-x^2)^n\,. \tag{3.56}$$

Plugging this into (3.55), we see that it gives us

$$C_n = \frac{2n-1}{2n}\,C_{n-1} + \frac{(2n-1)!}{2^{2n}\,(n!)^2}\,\int_{-1}^1 x\,d[(1-x^2)^n]\,. \tag{3.57}$$

Integrating the last term by parts gives us

$$C_n = \frac{2n-1}{2n}\,C_{n-1} - \frac{1}{2n}\,C_n\,, \tag{3.58}$$

which implies that

$$(2n+1)\,C_n = (2n-1)\,C_{n-1}\,. \tag{3.59}$$

This means that $(2n+1)\,C_n$ is *independent of* n, and so it must be that $(2n+1)\,C_n = C_0$. At last we have something easy to evaluate, since (3.55) implies that

$$C_0 = \int_{-1}^{1} dx\; = 2\,. \tag{3.60}$$

Thus, finally, we arrive at $C_n = 2/(2n+1)$, and so the normalisation of the integral of $[P_n(x)]^2$ is established:

$$\int_{-1}^{1} dx [P_n(x)]^2 = \frac{2}{2n+1}\,. \tag{3.61}$$

Let us review what we have achieved. Starting from a proposed expansion of an arbitrary function $f(x)$ as a sum of Legendre polynomials as in (3.29);

$$f(x) = \sum_{\ell\ge 0} a_\ell\, P_\ell(x)\,, \tag{3.62}$$

we have now found that the expansion coefficients a_ℓ are give by

$$a_\ell = \tfrac{1}{2}(2\ell+1)\int_{-1}^{1} dx\, f(x)\, P_\ell(x)\,. \tag{3.63}$$

It is time to look at a few examples. First, we may note that it is often very helpful to use Rodrigues' formula in order to evaluate the integral (3.63). Substituting (3.39) into (3.63), and integrating by parts, we obtain

$$a_\ell = \frac{(2\ell+1)}{2^{\ell+1}\,\ell!}\Big[\frac{d^{\ell-1}}{dx^{\ell-1}}\,(x^2-1)^\ell\Big]_{-1}^{1} - \frac{(2\ell+1)}{2^{\ell+1}\,\ell!}\int_{-1}^{1} dx\, f'(x)\,\frac{d^{\ell-1}}{dx^{\ell-1}}\,(x^2-1)^\ell\,. \tag{3.64}$$

The boundary term gives zero, since the $(\ell-1)$'th derivative of $(x^2-1)^\ell$ leaves one overall factor of (x^2-1), and this vanishes at $x=\pm 1$. Continuing this procedure, we can perform $(\ell-1)$ further integrations by parts, ending up with

$$a_\ell = \frac{(2\ell+1)}{2^{\ell+1}\,\ell!}\int_{-1}^{1} dx\,\frac{d^\ell f(x)}{dx^\ell}\,(1-x^2)^\ell\,. \tag{3.65}$$

Notice in particular that if the given function $f(x)$ is itself a polynomial of degree n, then all its derivatives $d^\ell f(x)/dx^\ell$ for $\ell > n$ vanish. This means that the all the expansion coefficients a_ℓ will vanish for $\ell > n$. This should not be a surprise, since we know that $P_\ell(x)$ is itself a polynomial of degree ℓ. In fact the set of Legendre polynomials with $0 \le \ell \le n$

really form a basis for the set of all possible polynomials of degree $\le n$. For example, we have

$$P_0(x) = 1\,, \qquad P_1(x) = x\,, \qquad P_2(x) = \tfrac{1}{2}(3x^2 - 1)\,, \tag{3.66}$$

and we can see just by doing elementary algebra that we can re-express the general quadratic polynomial $a\,x^2 + b\,x + c$ as

$$a\,x^2 + b\,x + c = (c + \tfrac{1}{3}a)\,P_0(x) + b\,P_1(x) + \tfrac{2}{3}a\,P_2(x)\,. \tag{3.67}$$

It is clear that we can do a similar expansion for any polynomial of finite degree n, and (3.65) gives us the expressions for the coefficients a_ℓ, which will be non-zero only for $\ell \le n$.

More generally, if the function $f(x)$ that we are expanding is non-polonomial in x, we shall get an infinite series in (3.62).

3.3 Azimuthally-symmetric solutions of Laplace's equation

Having constructed the Legendre polynomials, and determined their orthogonality and normalisation properties, we can now use them in order to construct azimuthally-symmetric solutions of the Laplace or Helmholtz equations. (We shall move on to case without azimuthal symmetry later.)

Recall, from section 2.2, that if we consider functions that are independent of the azimuthal angle ϕ, then the solution $\psi(r,\theta,\psi)$ of the Laplace or Helmholtz equation was written as

$$\psi(r,\theta) = \frac{1}{r}\,R(r)\,\Theta(\theta)\,, \tag{3.68}$$

with Θ and R satisfying

$$\frac{1}{\sin\theta}\,\frac{d}{d\theta}\Big(\sin\theta\,\frac{d\Theta}{d\theta}\Big) + \lambda\,\Theta = 0 \tag{3.69}$$

and

$$\frac{d^2R}{dr^2} = \Big(\frac{\lambda}{r^2} - k^2\Big)\,R\,. \tag{3.70}$$

We determined that the functions $\Theta(\theta)$ will only be regular at the north and south poles of the sphere if $\lambda = \ell\,(\ell+1)$ where ℓ is an integer (which can be assumed non-negative, without loss of generality). The functions $\Theta(\theta)$ are then the Legendre polynomials, with $\Theta(\theta) \sim P_\ell(\cos\theta)$.

Let us specialise to the case of the Laplace equation, which means that $k = 0$ in the equation (3.70) for the radial function $R(r)$. It is easy to see that with $\lambda = \ell\,(\ell+1)$, the two independent solutions of (3.70) are

$$R \sim r^{\ell+1}\,, \qquad \text{and} \qquad R \sim r^{-\ell}\,. \tag{3.71}$$

It follows, therefore, that the most general azimuthal solution of the Laplace equation $\nabla^2 \psi = 0$ in spherical polar coordinates can be written as

$$\psi(r,\theta) = \sum_{\ell\ge 0} (A_\ell\, r^\ell + B_\ell\, r^{-\ell-1})\, P_\ell(\cos\theta)\,. \tag{3.72}$$

We established the orthogonality relations for the Legendre polynomials, given in (3.30) and (3.31) with C_ℓ eventually determined to be $C_\ell = 2/(2\ell+1)$. In terms of θ, related to x by $x = \cos\theta$, we therefore have

$$\int_0^\pi \sin\theta\, d\theta\, P_\ell(\cos\theta)\, P_n(\cos\theta) = \frac{2}{2\ell+1}\,\delta_{\ell n}\,, \tag{3.73}$$

The δ symbol on the right-hand side here is the *Kronecker delta* function. By definition, δ_{mn} is zero if $m \ne n$, while it equals 1 if $m = n$. Thus (3.73) says that the integral on the left-hand side vanishes unless $\ell = n$, in which case it gives $2/(2\ell+1)$.

We can use these results in order to solve problems in potential theory. Suppose, for example, the electrostatic potential is specified everywhere on the surface of a sphere of radius a, as $\psi(a,\theta) = V(\theta)$ for some given function $V(\theta)$, and that we wish to calculate the potential $\psi(r,\theta)$ everywhere outside the sphere. Since the potential must die off, rather than diverge, as r tends to infinity, it follows that the coefficients A_ℓ in (3.72) must be zero, and so our solution is of the form

$$\psi(r,\theta) = \sum_{\ell\ge 0} B_\ell\, r^{-\ell-1}\, P_\ell(\cos\theta)\,. \tag{3.74}$$

To determine the remaining coefficients B_ℓ, we set $r = a$ and use the given boundary data $\psi(a,\theta) = V(\theta)$:

$$\psi(a,\theta) = V(\theta) = \sum_{\ell\ge 0} B_\ell\, a^{-\ell-1}\, P_\ell(\cos\theta)\,. \tag{3.75}$$

Multiplying by $P_n(\cos\theta)$ and integrating over $\int \sin\theta\, d\theta$, we get

$$\int_0^\pi \sin\theta\, d\theta\, V(\theta)\, P_n(\cos\theta) = \frac{2}{2n+1}\, a^{-n-1}\, B_n\,, \tag{3.76}$$

whence

$$B_n = \tfrac{1}{2}(2n+1)\, a^{n+1} \int_0^\pi \sin\theta\, d\theta\, V(\theta)\, P_n(\cos\theta)\,. \tag{3.77}$$

Given $V(\theta)$, we can calculate the coefficients B_n.

Suppose, for example, we are given that $V(\theta)$ is $+V$ for $0 \le \frac{1}{2}\pi$, and $V(\theta)$ is $-V$ for $\frac{1}{2}\pi < \theta \le \pi$, where V is a constant. The integral in (3.77) can be evaluated fairly straightforwardly using Rodrigues' formula (3.39), leading to the conclusion that B_ℓ is zero if ℓ is even, while

$$B_\ell = (-2)^{-(\ell-1)/2} \, \frac{(2\ell+1)\,(\ell-2)!! \; a^{\ell+1}}{2\Big(\frac{1}{2}(\ell+1)\Big)!} \tag{3.78}$$

when ℓ is odd. (Note that $(2p+1)!!$ means $(2p+1)(2p-1)(2p-3)\cdots \times 5 \times 3 \times 1$.) The first few terms in the solution give

$$\psi(r,\theta) = V\,\Big[\frac{3a^2}{2r^2}\,P_1(\cos\theta) - \frac{7a^4}{8r^4}\,P_3(\cos\theta) + \frac{11a^6}{16r^6}\,P_5(\cos\theta) + \cdots\Big]\,. \tag{3.79}$$

3.4 The generating function for the Legendre polynomials

There is yet another way to define the Legendre polynomials, which is very useful in its own right. This is via what is called a *Generating Function.* The claim is that

$$G(x,t) \equiv (1-2x\,t+t^2)^{-1/2} = \sum_{\ell\ge 0} t^\ell\, P_\ell(x)\,, \tag{3.80}$$

where, for convergence of the series, we must have $|t|<1$. How do we use this to read off the Legendre polynomials? We perform a power series expansion of the left-hand side, in increasing powers of t. Doing this, we find that the left-hand side gives

$$1 + x\,t + \tfrac{1}{2}(3x^2-1)\,t^2 + \tfrac{1}{2}(5x^3-3x)\,t^3 + \tfrac{1}{8}(35x^4-30x^2+3)\,t^4 + \cdots\,. \tag{3.81}$$

Equating this with the right-hand side of (3.80), and comparing the coefficients of each power of t, we read off

$$P_0(x)=1\,,\quad P_1(x)=x\,,\quad P_2(x)=\tfrac{1}{2}(3x^2-1)\,,\quad P_3(x)=\tfrac{1}{2}(5x^3-3x) \tag{3.82}$$

and so on, which is precisely what we were finding in (3.26).

Now let's check that *all* the coefficient functions $P_\ell(x)$ in (3.80) are indeed the Legendre polynomials. One way to do this is to slog out an explicit power-series expansion of the left-hand side in (3.80), and then to show that by equating the coefficients of each power of t with those on the right-hand side, we can recognise the power-series expansion of $P_\ell(x)$ that we already know. This is done in detail below. A more elegant approach, however, is as follows. We want to show that all the $P_\ell(x)$ defined by (3.80) satisfy the Legendre equation

$$(1-x^2)\,P_\ell'' - 2x\,P_\ell' + \ell(\ell+1)\,P_\ell = 0\,. \tag{3.83}$$

Multiplying by t^ℓ and summing, this is equivalent to showing that

$$H \equiv \sum_{\ell\ge 0} t^\ell\,[(1-x^2)\,P_\ell'' - 2x\,P_\ell' + \ell(\ell+1)\,P_\ell] \tag{3.84}$$

is equal to zero. Now, looking at (3.80) we can see that H can be written as

$$H = (1-x^2)\,\frac{\partial^2 G(x,t)}{\partial x^2} - 2x\,\frac{\partial G(g,t)}{\partial x} + t\,\frac{\partial^2 (t\,G(x,t))}{\partial t^2}\,. \tag{3.85}$$

(The three terms here correlate exactly with the three terms in H.) It is now just a simple exercise in differentiation to show that indeed we have $H=0$, which proves that the functions $P_\ell(x)$ defined by (3.80) satisfy the Legendre equation. They are clearly polynomials, because the power-series expansion of the left-hand side of (3.80) in powers of t will clearly have x-dependent coefficients that are polynomial in x. (See below, if you doubt this.)

Finally, we must check the normalisation, i.e. that $P_\ell(1)=1$. This is very easy; we just set $x=1$ in (3.80), to get

$$(1-2t+t^2)^{-1/2} = \sum_{\ell\ge 0} t^\ell\, P_\ell(1)\,. \tag{3.86}$$

But the left-hand side is just $(1-t)^{-1}$, which has the binomial expansion

$$\frac{1}{1-t} = 1+t+t^2+t^3+t^4+\cdots = \sum_{\ell\ge 0} t^\ell\,, \tag{3.87}$$

and so by comparing with the right-hand side in (3.86) we immediately get $P_\ell(1)=1$.

To finish off this discussion, here is a different, and rather ponderous, direct proof that the generating function (3.80) gives exactly the same Legendre polynomials as the $P_\ell(x)$ defined by Rodrigues' formula (3.39), for all ℓ. To do this, first take the generating function in (3.80) and use the binomial theorem

$$(1+z)^\alpha = 1+\alpha\, z + \frac{\alpha\,(\alpha-1)}{2!}\, z^2 + \cdots \tag{3.88}$$

to expand the left-hand side in powers of $(-2x\,t+t^2)$. For $\alpha=-\frac{1}{2}$ (3.88) can easily be seen to be expressible as

$$(1+z)^{-1/2} = \sum_{n\ge 0} \frac{(-1)^n\,(2n)!}{2^{2n}\,(n!)^2}\, z^n\,, \tag{3.89}$$

and so we get

$$(1-2x\,t+t^2)^{-1/2} = \sum_{n\ge 0} \frac{(2n)!}{2^{2n}\,(n!)^2}\,(2x\,t-t^2)^n\,. \tag{3.90}$$

Next we expand the factor $(2x\,t-t^2)^n$ using the binomial theorem, for which a convenient formulation is

$$(a+b)^n = \sum_{k=0}^n \begin{pmatrix} n\\ k\end{pmatrix}\, a^{n-k}\, b^k\,. \tag{3.91}$$

This now gives us a double series,

$$(1-2x\,t+t^2)^{-1/2} = \sum_{n\ge 0} \frac{(2n)!}{2^{2n}\,(n!)^2}\,t^n\,\sum_{k=0}^{n}(-1)^k \begin{pmatrix} n\\ k\end{pmatrix} (2x)^{n-k}\,t^k\,,$$
$$= \sum_{n\ge 0}\sum_{k=0}^{n}(-1)^k\,\frac{(2n)!}{2^{2n}\,n!\,k!\,(n-k)!}\,(2x)^{n-k}\,t^{n+k}\,. \qquad (3.92)$$

We are almost there, but one further manipulation on the expression (3.92) is needed. There are many ways of reorganising the summation of terms in a double series, and for our present purposes the one we need is the following:

$$\sum_{n\ge 0}\sum_{k=0}^{n} a(k,n-k) = \sum_{r\ge 0}\sum_{s=0}^{[r/2]} a(s,r-2s)\,, \qquad (3.93)$$

where $[r/2]$ means the integer part of $r/2$. (Exercise: Check this!). The bottom line is that, after finally relabelling the summation variables, the expression (3.92) can be turned into another expression, namely

$$(1-2x\,t+t^2)^{-1/2} = \sum_{n\ge 0}\sum_{k=0}^{[n/2]}(-1)^k\,\frac{(2n-2k)!}{2^{2n-2k}\,k!\,(n-k)!\,(n-2k)!}\,(2x)^{n-2k}\,t^n\,. \qquad (3.94)$$

We appeared just to have exchanged one expression that resembles a dog's breakfast for another, but the point now is that (3.94) brings us back (finally!) to our expression from Rodrigues' formula (3.39). From (3.44) and (3.47), we can see, after a simple redefinition of the k summation variable, that the thing that multiplies the coefficient of t^n in (3.94) is nothing but our old friend $P_n(x)$, as defined by Rodrigues' formula (3.39). Thus the equivalence of the two definitions for $P_\ell(x)$, from Rodrigues' formula (3.39) and the generating function (3.80) is established.

3.5 The associated Legendre functions

In our analysis in section 3, we made the specialisation from the Associated Legendre Equation (2.28) to the case of the Legendre Equation, where $m=0$. Let us now return to the full Associated Legendre Equation, which we shall need for finding general solutions of Laplace's equation, in which the potential function is allowed to depend on the azimuthal angle ϕ. For convenience, we present again the Associated Legendre Equation:

$$\frac{d}{dx}\Big((1-x^2)\,\frac{dy}{dx}\Big) + \Big(\lambda - \frac{m^2}{1-x^2}\Big)\,y = 0\,. \qquad (3.95)$$

As mentioned previously, it turns out that we can construct the relevant solutions of this equation rather simply, in terms of the Legendre polynomials that we have already studied.

To begin, we write $y = (1-x^2)^{m/2}\, w$, and substitute this into (3.95). After simple algebra we find, after extracting an overall factor of $(1-x^2)^{m/2}$, that w must satisfy

$$(1-x^2)\, w'' - 2(m+1)\, x\, w' + [\lambda - m\,(m+1)]\, w = 0\,. \tag{3.96}$$

(We are using a prime to denote differentiation d/dx here.) Now suppose that we have a solution u of the ordinary Legendre equation:

$$(1-x)^2\, u'' - 2x\, u' + \lambda\, u = 0\,. \tag{3.97}$$

Next, we differentiate this m times. Let us use the notation ∂^m as a shorthand for d^m/dx^m. It is useful to note that we have the following lemma, which is just a consequece of Leibnitz' rule for the differentiation of a product, iterated m times:

$$\begin{aligned}\partial^m(f\,g) &= f\,(\partial^m g) + m\,(\partial f)\,(\partial^{m-1} g) + \frac{m(m-1)}{2!}\,(\partial^2 f)\,(\partial^{m-2} g) \\ &\quad + \frac{m(m-1)(m-2)}{3!}\,(\partial^3 f)\,(\partial^{m-3} g) + \cdots\,.\end{aligned} \tag{3.98}$$

We only need the first two or three terms in this expression if we apply it to the products in (3.97), and so we easily find that

$$(1-x^2)\,\partial^{m+2} u - 2(m+1)\, x\,\partial^{m+1} u + [\lambda - m(m+1]\,\partial^m\, u = 0\,. \tag{3.99}$$

Thus we see that setting $w = \partial^m u$, we have constructed a solution of (3.96) in terms of a solution u of the Legendre equation (3.97). The upshot, therefore, is that if we define

$$P_\ell^m(x) \equiv (-1)^m\,(1-x^2)^{m/2}\,\frac{d^m}{dx^m}\,P_\ell(x)\,, \tag{3.100}$$

where $P_\ell(x)$ is a Legendre polynomial, then $P_\ell^m(x)$ will be a solution of the Associated Legendre Equation with $\lambda = \ell\,(\ell+1)$:

$$\frac{d}{dx}\Big((1-x^2)\,\frac{dP_\ell^m}{dx}\Big) + \Big(\ell\,(\ell+1) - \frac{m^2}{1-x^2}\Big)\,P_\ell^m = 0\,. \tag{3.101}$$

Since $P_\ell(x)$ is regular everywhere including $x=\pm 1$, it is clear that $P_\ell^m(x)$ will be too. It is understood here that we are taking the integer m to be non-negative. It is clear that we must have $m \le \ell$ too, since if m exceeds ℓ then the m-fold derivative of the ℓ'th Legendre polynomial (which itself is of degree ℓ) will give zero.

Recall next that we have Rodrigues' formula (3.39), which gives us an expression for $P_\ell(x)$. Substituting this into (3.100), we get

$$P_\ell^m(x) = \frac{(-1)^m}{2^\ell\,\ell!}\,(1-x^2)^{m/2}\,\frac{d^{\ell+m}}{dx^{\ell+m}}\,(x^2-1)^\ell\,. \tag{3.102}$$

A nice little miracle now occurs: this formula makes sense for negative values of m too, provided that $m \geq -\ell$. Thus we have a construction of Associated Legendre Functions for all integers m in the interval $-\ell \leq m \leq \ell$.

Looking at the Associated Legendre Equation (3.101), we note that the equation itself is invariant under sending

$$m \longrightarrow -m\,, \tag{3.103}$$

since m appears only as m^2 in the equation. This means that if we take a solution with a given m, then sending m to $-m$ gives us another solution. What is more, only one solution at fixed ℓ and m^2 can be regular at $x = \pm 1$, since the second solution will have logarithmic singularities there (just like we saw for the Legendre functions). Since $P_\ell^m(x)$ and $P_\ell^{-m}(x)$ given by 3.102 are both regular at $x = \pm 1$, it follows therefore that they must be linearly dependent; i.e. $P_\ell^{-m}(x)$ must be some constant multiple of $P_\ell^m(x)$:

$$P_\ell^{-m}(x) = k\, P_\ell^m(x)\,. \tag{3.104}$$

It is easy to determine what the constant k is, by using (3.102). From (3.104) we get

$$\partial^{\ell-m}(x^2-1)^\ell = k\,(1-x^2)^m\,\partial^{\ell+m}(x^2-1)^\ell\,. \tag{3.105}$$

It is good enough just to look at the highest power of x, since all we need to do is to calculate what k is.[4] Thus we get

$$\frac{(2\ell)!}{(\ell+m)!}\,x^{\ell+m} = k\,(-1)^m\,x^{2m}\,\frac{(2\ell)!}{(\ell-m)!}\,x^{\ell-m} \tag{3.106}$$

at the leading order in x, which fixes k and hence establishes that

$$P_\ell^{-m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!}\,P_\ell^m(x)\,. \tag{3.107}$$

Using this result we can now very easily work out the normalisation integral for the associated Legendre functions $P_\ell^m(x)$. The relevant integral we shall need to evaluate is

$$\int_{-1}^1 dx\, P_\ell^m(x)\, P_n^m(x)\,. \tag{3.108}$$

(It will become clear in section 3.6 why we have set the upper indices m equal here.) Using the same method as we used for the Legendre polynomials, it is easy to show that (3.108) vanishes unless $\ell = n$. For $\ell = m$, we can make use of (3.107) to write the required integral as

$$C_{\ell m} \equiv \int_{-1}^1 dx\,[P_\ell^m(x)]^2 = (-1)^m \frac{(\ell+m)!}{(\ell-m)!} \int_{-1}^1 dx\, P_\ell^m(x)\, P_\ell^{-m}(x)\,. \tag{3.109}$$

[4]One could, more adventurously, give another proof that $P_\ell^{-m}(x)$ and $P_\ell^m(x)$ are linearly dependent by checking *all* powers of x. We leave this as an exercise for the reader.

Our task is to calculate the constants $C_{\ell m}$. We can use the generalised Rodrigues formula (3.102), thus giving

$$C_{\ell m} = \frac{(-1)^m\,(\ell+m)!}{2^{2\ell}\,(\ell!)^2\,(\ell-m)!}\int_{-1}^{1} dx\,\partial^{\ell+m}(x^2-1)^\ell\,\partial^{\ell-m}(x^2-1)^\ell\,. \tag{3.110}$$

(Note that by making use of (3.107) we have managed to get the two powers of $(1-x^2)^{m/2}$ that would otherwise have arisen from $(P_\ell^m)^2$ to cancel instead of adding, which simplifies life considerably.) Integrating by parts $\ell+m$ times in (3.110), and noting that the boundary terms all give zero, we therefore have

$$\begin{aligned} C_{\ell m} &= \frac{(\ell+m)!}{2^{2\ell}\,(\ell!)^2\,(\ell-m)!}\int_{-1}^{1} dx\,(1-x^2)^\ell\,\partial^{2\ell}(x^2-1)^\ell\,,\\ &= \frac{(2\ell)!\,(\ell+m)!}{2^{2\ell}\,(\ell!)^2\,(\ell-m)!}\int_{-1}^{1} dx\,(1-x^2)^\ell\,. \end{aligned} \tag{3.111}$$

The integral here is the same one we had to evaluate in the case of the Legendre polynomials in (3.55); the only difference now is the extra factorial prefactors. Thus from the previous results in section 3.2, we see that

$$C_{\ell m} = \frac{2}{2\ell+1}\,\frac{(\ell+m)!}{(\ell-m)!}\,. \tag{3.112}$$

In other words, we have shown that

$$\int_{-1}^{1} dx\,P_\ell^m(x)\,P_{\ell'}^m(x) = \frac{2}{2\ell+1}\,\frac{(\ell+m)!}{(\ell-m)!}\,\delta_{\ell\ell'}\,. \tag{3.113}$$

3.6 The spherical harmonics and Laplace's equation

It may be recalled that a while back, we were solving equations such as the Laplace equation or the Helmholtz equation in spherical polar coordinates, in section 2.2. We had reduced the problem, by means of separating variables, to solving for the radial functions $R(r)$ and the functions $Y(\theta,\phi)$ on the spherical constant-radius surfaces. Thus the Helmholtz equation $\nabla^2\,\psi + k^2\,\psi = 0$ implied that if we write

$$\psi(r,\theta,\phi) = \frac{1}{r}\,R(r)\,Y(\theta,\phi)\,, \tag{3.114}$$

the $R(r)$ and $Y\theta,\phi)$ should satisfy

$$\nabla^2_{(\theta,\phi)}\,Y = -\lambda\,Y\,,\qquad \frac{d^2R}{dr^2} = \Big(\frac{\lambda}{r^2} - k^2\Big)\,R\,, \tag{3.115}$$

where

$$\nabla^2_{(\theta,\phi)} \equiv \frac{1}{\sin\theta}\,\frac{\partial}{\partial\theta}\Big(\sin\theta\,\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\,\frac{\partial^2}{\partial\phi^2} \tag{3.116}$$

is the Laplace operator on the unit sphere. We then performed the further separation of angular variables on the sphere, with $Y(\theta,\phi) = \Theta(\theta)\,\Phi(\phi)$, showing that for regularity we must have $\lambda = \ell\,(\ell+1)$, and m is an integer with $-\ell \le m \le \ell$.

Putting together what we found for the angular functions, we see that the $Y(\theta,\phi)$ are characterised by the two integers ℓ and m, and we may define

$$Y_{\ell m}(\theta,\phi) \equiv \sqrt{\frac{(2\ell+1)}{4\pi}}\,\sqrt{\frac{(\ell-m)!}{(\ell+m)!}}\,P_\ell^m(\cos\theta)\,e^{\mathrm{i}\,m\,\phi}\,,\qquad \ell \ge 0\,,\quad -\ell \le m \le \ell\,. \tag{3.117}$$

The *Spherical Harmonics* $Y_{\ell m}(\theta,\phi)$ satisfy

$$-\nabla^2_{(\theta,\phi)}\,Y_{\ell m}(\theta,\phi) = \ell\,(\ell+1)\,Y_{\ell m}(\theta,\phi)\,. \tag{3.118}$$

These spherical harmonics form the complete set of regular solutions of $\nabla^2_{(\theta,\phi)}\,Y = -\lambda\,Y$ on the unit sphere. Note from (3.107) that we have

$$Y_{\ell,-m}(\theta,\phi) = (-1)^m\,\bar Y_{\ell m}(\theta,\phi)\,, \tag{3.119}$$

where the bar denotes complex conjugation.

From our results in the previous sections, we can easily see that the spherical harmonics satsify the orthogonality properties

$$\int d\Omega\,\bar Y_{\ell' m'}(\theta\,\phi)\,Y_{\ell m}(\theta,\phi) = \delta_{\ell\ell'}\,\delta_{mm'}\,, \tag{3.120}$$

where

$$d\Omega \equiv \sin\theta\,d\theta\,d\phi \tag{3.121}$$

is the area element on the unit sphere, and $\int d\Omega\,X$ means

$$\int_0^{2\pi} d\phi \int_0^\pi \sin\theta\,d\theta\,X\,. \tag{3.122}$$

Thus (3.120) just says that the integral on the left-hand side is zero unless $\ell' = \ell$ and $m' = m$. Note that it is the integration over ϕ that is responsible for producing the Kronecker delta $\delta_{mm'}$, since the ϕ dependent factors in (3.120) are

$$\int_0^{2\pi} d\phi\,e^{\mathrm{i}\,(m-m')\,\phi}\,. \tag{3.123}$$

This integrates to zero if the integers m and m' are unequal, whilst giving 2π if $m = m'$. The remaining integration over θ in (3.120) then reduces, with m and m' equal, to the integral in (3.113), which then gives rise to the Kronecker delta function $\delta_{\ell\ell'}$ in (3.120).

It is instructive to look at the first few spherical harmonics explicitly. From (3.117), and using (3.102) to give the expressions for the P_ℓ^m, we find

$$
\begin{aligned}
Y_{0,0}(\theta,\phi) &= \frac{1}{\sqrt{4\pi}}\,,\\[2ex]
Y_{1,1}(\theta,\phi) &= -\sqrt{\frac{3}{8\pi}}\,\sin\theta\,e^{\mathrm{i}\,\phi}\,,\\
Y_{1,0}(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\,\cos\theta\,,\\
Y_{1,-1}(\theta,\phi) &= \sqrt{\frac{3}{8\pi}}\,\sin\theta\,e^{-\mathrm{i}\,\phi}\,,\\[2ex]
Y_{2,2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\,\sin^2\theta\,e^{2\mathrm{i}\,\phi}\,,\\
Y_{2,1}(\theta,\phi) &= -\sqrt{\frac{15}{8\pi}}\,\sin\theta\,\cos\theta\,e^{\mathrm{i}\,\phi}\,,\\
Y_{2,0}(\theta,\phi) &= \sqrt{\frac{5}{16\pi}}\,(3\cos^2\theta-1)\,,\\
Y_{2,-1}(\theta,\phi) &= \sqrt{\frac{15}{8\pi}}\,\sin\theta\,\cos\theta\,e^{-\mathrm{i}\,\phi}\,,\\
Y_{2,-2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\,\sin^2\theta\,e^{-2\mathrm{i}\,\phi}\,.
\end{aligned}
\tag{3.124}
$$

It is also instructive to rewrite the spherical harmonics in terms of Cartesian, rather than spherical polar, coordinates. Recall that the two coordinate systems are related by

$$x = r\,\sin\theta\,\cos\phi\,,\quad y = r\,\sin\theta sin\phi\,,\quad z = r\,\cos\theta\,. \tag{3.125}$$

We can write the expressions for x and y more succinctly in a single complex equation,

$$x + \mathrm{i}\,y = r\,\sin\theta\,e^{\mathrm{i}\,\phi}\,, \tag{3.126}$$

since we have the well-known result that $e^{\mathrm{i}\,\phi} = \cos\phi + \mathrm{i}\,\sin\phi$. Thus for the spherical harmonics listed in (3.124) we have

$$
\begin{aligned}
Y_{0,0} &= \frac{1}{\sqrt{4\pi}}\,,\\
Y_{1,1} &= -\sqrt{\frac{3}{8\pi}}\,\frac{x+\mathrm{i}\,y}{r}\,,\\
Y_{1,0} &= \sqrt{\frac{3}{4\pi}}\,\frac{z}{r}\,,\\
Y_{1,-1} &= \sqrt{\frac{3}{8\pi}}\,\frac{x-\mathrm{i}\,y}{r}\,,\\
Y_{2,2} &= \sqrt{\frac{15}{32\pi}}\,\frac{(x+\mathrm{i}\,y)^2}{r^2}\,,
\end{aligned}
$$

$$
\begin{aligned}
Y_{2,1} &= -\sqrt{\frac{15}{8\pi}}\,\frac{z\,(x+\mathrm{i}\,y)}{r^2}\,,\\
Y_{2,0} &= \sqrt{\frac{5}{16\pi}}\,\Big(\frac{3z^2}{r^2}-1\Big)=\sqrt{\frac{5}{16\pi}}\,\frac{2z^2-x^2-y^2}{r^2}\,,\\
Y_{2,-1} &= \sqrt{\frac{15}{8\pi}}\,\frac{z\,(x-\mathrm{i}\,y)}{r^2}\,,\\
Y_{2,-2} &= \sqrt{\frac{15}{32\pi}}\,\frac{(x-\mathrm{i}\,y)^2}{r^2}\,.
\end{aligned}
\tag{3.127}
$$

What we are seeing here is that for each value of ℓ, we are getting a set of functions, labelled by m with $-\ell \le m \le \ell$, that are all of the form of polynomials of degree ℓ in (x, y, z), divided by r^ℓ:

$$
Y_{\ell m} \sim \frac{x_{i_1}\, x_{i_2} \cdots x_{i_\ell}}{r^\ell}\,. \tag{3.128}
$$

The larger ℓ is, the larger the number of possible such polynomials. Looking at $\ell = 1$, we have in total three $Y_{1,m}$ functions, which could be reorganised, by taking appropriate linear combinations, as

$$
\frac{x}{r}\,, \qquad \frac{y}{r}\,, \qquad \frac{z}{r}\,. \tag{3.129}
$$

Thus once we know one of them, the other two just correspond to rotating the coordinate system through 90 degrees about one or another axis. The same is true of all the higher harmonics too. The spherical harmonics thus have built into them the "knowledge" of the rotational symmetries of the sphere. Our procedure for deriving the spherical harmonics was completely "non-transparent," in the sense that no explicit use of the rotational symmetry of the sphere was made in the derivation. But at the end of the day, we see that the harmonics we have obtained do indeed reflect the symmetries. In the language of group theory, one says that the spherical harmonics $Y_{\ell m}$ fall into representations of the rotation group. One of the rather remarkable "miracles" that we encountered during our derivation, namely that the solutions to the associated Legendre equation could be constructed from solutions of the ordinary Legendre equation, ultimately has its explanation in the fact that the harmonics $Y_{\ell m}$ with $m \ne 0$ are simply related to the $m = 0$ harmonic $Y_{\ell 0}$ by symmetry rotations of the sphere.

Going back to our general form of the separated solution (3.114), and noting that if we are solving Laplace's equation then the radial functions still satisfy (2.24) with $k = 0$, just as they did in the azimuthally-symmetric case $m = 0$, we now have that the most general solution of Laplace's equation in spherical polar coordinates[5] is written as

$$\psi(r,\theta,\phi) = \sum_{\ell\ge 0}\sum_{m=-\ell}^{\ell} (A_{\ell m}\, r^\ell + B_{\ell m}\, r^{-\ell-1})\, Y_{\ell m}(\theta,\phi)\,. \tag{3.130}$$

The constants $A_{\ell m}$ and $B_{\ell m}$, which depend on both ℓ and m, are as yet arbitrary. Their values are determined by boundary conditions, as in the previous potential-theory examples that we have looked at. Because we are now allowing the azimuthal separation constant m to be non-zero, the class of solutions described by (3.130) includes those that are dependent on the azimuthal angle θ.

Let us conclude this part of the discussion with a simple example. Suppose the electrostatic potential is given on the the spherical surface $r=a$, and that one is told that

$$\psi(a,\theta,\phi) = V(\theta,\phi) \tag{3.131}$$

on this surface, for some given function $V(\theta,\phi)$. Calculate the potential everywhere inside the surface.

First, we note that since the potential must remain finite as r approaches zero, it must be that all the coefficients $B_{\ell m}$ in (3.130) vanish in this problem. The $A_{\ell m}$ can be calculated by setting $r=a$ in what remains in (3.130), and then multiplying by $\bar Y_{\ell',m'}(\theta,\phi)$ and integrating over the sphere;

$$\int d\Omega\, \psi(a,\theta,\phi)\, \bar Y_{\ell'}^{m'}(\theta,\phi) = a^{\ell'}\, A_{\ell' m'}\,. \tag{3.132}$$

Here, we have made use of the orthogonality relations (3.120). Thus we have

$$A_{\ell m} = a^{-\ell}\int d\Omega\, V(\theta,\phi)\, \bar Y_{\ell m}(\theta,\phi) \tag{3.133}$$

Suppose now, as an example, that we are given that

$$V(\theta,\phi) = V_0\, \sin\theta\, \sin\phi\,, \tag{3.134}$$

where V_0 is a constant. Becaiuse this potential has a particularly simply form, we can spot that it can be written in terms of the spherical harmonics as

$$V_0\, \sin\theta\, \sin\phi = \frac{1}{2\mathrm{i}}\, V_0\, \sin\theta\, (e^{\mathrm{i}\phi} - e^{-\mathrm{i}\,\phi}) = \mathrm{i}\sqrt{\frac{2\pi}{3}}\, V_0\, (Y_{1,1}(\theta,\phi) + Y_{1,-1}(\theta,\phi))\,, \tag{3.135}$$

where we have used the $\ell=0$ expressions in (3.124). This, of course, is all one is really doing in any case, when one uses the orthogonality relations to determine the expansion

[5] That is, the most general solution that is regular on the spherical surfaces at constant r.

coefficients; we just need to figure out what linear combination of the basis functions constructs for us the desired function. It just happens in this example that the answer is so simple that we can spot it without doing all the work of evaluating the integrals in (3.135). Thus, we see by comparing with the general solution (3.130) that we must have

$$\psi(r,\theta,\phi) = \mathrm{i}\sqrt{\frac{2\pi}{3}}\, V_0\, \frac{r}{a}\, (Y_{1,1}(\theta,\phi) + Y_{1,-1}(\theta,\phi))\,. \tag{3.136}$$

This is actually real (as it must be) despite the presence of the i, since the $Y_{\ell m}$ functions themselves are complex. In fact in this example it is obviously much simpler to write the answer explicitly, using the expressions in (3.124); we just get

$$\psi(r,\theta,\phi) = \frac{r}{a}\, V_0\, \sin\theta\, \sin\phi\,. \tag{3.137}$$

The example chosen here was so simple that it perhaps makes the use of the whole edifice of spherical harmonic expansions look a trifle superfluous. The principles involved in this example, though, are no different from the ones that would be involved in a more complicated example.

3.7 Another look at the generating function

Before moving on, let us return to the generating function for the Legendre polynomials, defined in (3.80). There is a nice physical interpretation of this construction, which we shall now describe. In the process, we shall illustrate another very useful technique that can sometimes be used in order to determine the coeeficients in the expansion of the solution of Laplace's equation in terms of Legendre polynomials or spherical harmonics.

Consider the problem of a charge of unit strength, sitting on the z axis at a point $z = r'$. We know, since it is an axially-symmetric situation, that the potential must be expressible as

$$\phi(r,\theta) = \sum_{\ell\ge 0} (A_\ell\, r^\ell + B_\ell\, r^{-\ell-1})\, P_\ell(\cos\theta)\,. \tag{3.138}$$

To determine the coefficients, we must first make a choice between considering either the region where $r \ge r'$, or the region where $r \le r'$.

In the region $r \ge r'$, we will require that ψ tend to zero as $r \to \infty$; it should not blow up at large r, because there is no other charge in the problem that would make it do so. (Of course we could allow it to tend to an arbitrary constant value at infinity, but that is a trivial issue, since one only ever measures potential differences, and so without loss of generality (wolog, for short!) we can assume the constant asymptotic value is zero.) Thus boundary conditions in the problem determine that

$$A_\ell = 0\,, \qquad \ell \ge 0\,. \tag{3.139}$$

What about the remaining constants B_ℓ? We don't have a specific boundary anywhere that will determine these, but we do have the following simple way to work them out. Consider the potential *on axis*, i.e. on the z axis, which for $z > 0$ means $\theta = 0$. Since we are looking at the region $r > r'$, the on-axis potential is therefore given by

$$\psi(r,0) = \frac{1}{r - r'}\,. \tag{3.140}$$

(For simplicity we use units where the $4\pi\,\epsilon_0$ that appears in the rather cumbersome SI system of units has been absorbed.) Now we can determine the constants B_ℓ by matching this to the general solution (3.138) (with $A_\ell = 0$, of course, since we have already established that). Thus we shall have

$$\frac{1}{r - r'} = \sum_{\ell\ge 0} B_\ell\, r^{-\ell-1}\, P_\ell(1)\,. \tag{3.141}$$

We can pull out a factor of $1/r$ on the left-hand side, and do a binomial expansion of $(1 - r'/r)^{-1} = 1 + r'/r + (r'/r)^2 + \cdots$ (noting that $r'/r < 1$, since $r > r'$, and so the series converges):

$$\frac{1}{r}\sum_{\ell\ge 0}\Big(\frac{r'}{r}\Big) = \sum_{\ell\ge 0} B_\ell\, r^{-\ell-1}\,. \tag{3.142}$$

We have also used that $P_\ell(1) = 1$. Equating coefficients of each power of r in (3.142), we find $B_\ell = r'^\ell$. Thus from (3.138), the general solution at a point (r,θ) with $r > r'$ is given by

$$\psi(r,\theta) = \sum_{\ell\ge 0}\frac{r'^\ell}{r^{\ell+1}}\, P_\ell(\cos\theta)\,, \qquad r > r'\,. \tag{3.143}$$

This gives the potential at a point (r,θ) (for arbitrary azimuthal angle ϕ, of course, since the configuration is axially symmetric), due to a unit charge at $z = r'$ on the z axis.

To make contact with the generating function, we now observe that we can in fact write down the solution to this problem in closed form. The potential $\psi(r,\theta)$ will just be the inverse of the distance from the point (r,θ) to the point $z = r'$ on the z axis where the unit charge is located. Using the cosine rule, this distance is $(r^2 - 2r\,r'\,\cos\theta + r'^2)^{1/2}$. Thus from (3.143) it must be that

$$(r^2 - 2r\,r'\,\cos\theta + r'^2)^{-1/2} = \sum_{\ell\ge 0}\frac{r'^\ell}{r^{\ell+1}}\, P_\ell(\cos\theta)\,. \tag{3.144}$$

Pulling out a factor of r^2 from the bracket on the left-hand side, and defining $t \equiv r'/r$, $x \equiv \cos\theta$, we see that (3.144) is nothing but

$$(1 - 2x\,t + t^2)^{-1/2} = \sum_{\ell \ge 0} t^\ell\, P_\ell(x)\,. \tag{3.145}$$

This is precisely the generating function (3.80).

It is straightforward to repeat the above exercise for the region where $r < r'$. Here, of course, we instead deduce from the requirement that the potential be regular at $r = 0$ that we must have $B_\ell = 0$ for all ℓ. This time, it is the coefficients A_ℓ that are non-zero, and they can be determined by matching the general solution (3.138) to the on-axis solution $\psi(r, 0) = 1/(r' - r)$. This time, one must pull out a factor of r' in the denominator, and expand the on-axis potential as $1/(r' - r) = r'^{-1}\,(1 + r/r' + (r/r')^2 + \cdots)$, since now it is r'/r that is less than one, and thus leads to a convergent series. Thus in the region $r < r'$ we find the potential is given by

$$\psi(r, \theta) = \sum_{\ell \ge 0} \frac{r^\ell}{r'^{\ell+1}}\, P_\ell(\cos\theta)\,, \qquad r < r'\,, \tag{3.146}$$

rather than (3.143).

As well as providing a physical interpretation of the generating function, in this subsection we have illustrated another useful technique in the armoury of tools for solving equations such as Laplace's equation. Namely, if one has found the general solution, and if one can easily work out the solution on the z axis, then by matching coefficients on the z axis, one has then determined the solution everywhere. In the example discussed here, we could rather easily solve the problem off-axis too, but in more complicated situations the technique can be very powerful.

Finally, we note that there is a generalisation of (3.144) that can be given, in which the unit charge is located at an arbitrary point. This is therefore an expression for

$$\psi = \frac{1}{|\vec r - \vec r\,'|}\,, \tag{3.147}$$

the potential at position vector $\vec r$, due to a point charge at $\vec r\,'$. Without too much difficulty, one can show that it is expressible as a sum over spherical harmonics. As usual, there are two different expressions, depending upon whether $r > r'$ or $r < r'$, where $r \equiv |\vec r|$, $r' \equiv |\vec r\,'|$. We have:

$$r > r' : \qquad \frac{1}{|\vec r - \vec r\,'|} = \sum_{\ell \ge 0} \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell + 1}\, \frac{r'^\ell}{r^{\ell+1}}\, \bar Y_{\ell m}(\theta', \phi')\, Y_{\ell m}(\theta, \phi)\,, \tag{3.148}$$

$$r < r' : \qquad \frac{1}{|\vec r - \vec r\,'|} = \sum_{\ell \ge 0} \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell + 1}\, \frac{r^\ell}{r'^{\ell+1}}\, \bar Y_{\ell m}(\theta', \phi')\, Y_{\ell m}(\theta, \phi)\,, \tag{3.149}$$

where (r, θ, ϕ) denotes the point $\vec{r}$ in spherical polar coordinates, and likewise (r', θ', ϕ') denotes the point $\vec{r}'$. The proof of these formulae is by noting that since (3.147), viewed as a function of $\vec{r}$, is a solution of Laplace's equation, it must be expressible as a sum of the form (3.130). Then, by performing some manipulations in which one rotates to a coordinate system where $\vec{r}'$ lies along the rotated z axis, and invoking the previous result (3.144), the result follows after some simple algebra.

4 General Properties of Second-order ODE's

Consider the linear second-order ODE

$$y'' + p(x)\, y' + q(x)\, y = 0\,, \tag{4.1}$$

where the prime denotes a derivative with respect to x:

$$y' \equiv \frac{dy}{dx}\,, \qquad y'' \equiv \frac{d^2y}{dx^2}\,. \tag{4.2}$$

4.1 Singular points of the equation

First, we introduce the notion of singular points of the equation. A point $x = x_0$ is called an *ordinary point* if $p(x)$ and $q(x)$ are finite there.[6] The point $x = x_0$ is defined to be a *singular point* if either $p(x)$ or $q(x)$ diverges at $x = x_0$. For reasons that will become clear later, it is useful to refine this definition, and subdivide singular points into regular singular points, and irregular singular points. They are defined as follows:

- If either $p(x)$ or $q(x)$ diverges at $x = x_0$, but $(x - x_0)\, p(x)$ and $(x - x_0)^2\, q(x)$ remain finite, then $x = x_0$ is called a *regular singular point.*
- If $(x - x_0)\, p(x)$ or $(x - x_0)^2\, q(x)$ diverges at $x = x_0$, then $x = x_0$ is called an *irregular singular point.*

In other words, if the singularities are not too severe, meaning that a simple pole in $p(x)$ is allowed, and a double pole in $q(x)$ is allowed, then the singularity is a "regular" one. As

[6] In this course we shall always use the word "finite" in its proper sense, of meaning "not infinite." Some physicists have the tiresome habit of misusing the term to mean (sometimes, but not always!) "non-zero," which can cause unnecessary confusion. (As in, for example, *The heat bath had a finite temperature*, or *There is a finite probability of winning the lottery.*) Presumably, however, these same people would not disagree with the mathematical fact that if x and y are finite numbers, then $x + y$ is a finite number too. Their inconsistency is then apparent if one considers the special case $x = 1, y = -1$. We shall have further comments on linguistics later...

we shall see, equations whose only singular points are regular ones admit better-behaved series solutions than those with irregular singular points.

As stated above, these definitions apply only for finite values of x_0. To analyse the point $x=\infty$, we can first perform the change of independent variable from x to $z=1/x$, and study the behaviour of the transformed equation at $z=0$. Using the chain rule to write

$$\frac{d}{dx}=z'\,\frac{d}{dz}=-z^2\,\frac{d}{dz}\,,\qquad \frac{d^2}{dx^2}=z'^2\,\frac{d^2}{dz^2}+z''\,\frac{d}{dz}=z^4\,\frac{d^2}{dz^2}+2z^3\,\frac{d}{dz}\,, \tag{4.3}$$

where $z'\equiv dz/dx$, we see that the equation (4.1) becomes, with y, p and q now viewed as $y(1/z)$, $p(1/z)$ and $q(1/z)$,

$$\frac{d^2y}{dz^2}+\frac{(2z-p)}{z^2}\,\frac{dy}{dz}+\frac{q}{z^4}\,y=0\,. \tag{4.4}$$

The point $x=\infty$ is therefore an ordinary point if $\tilde p\equiv\frac{(2z-p)}{z^2}$ and $\tilde q\equiv\frac{q}{z^4}$ are finite at $z=0$; it is a regular singular point if $\tilde p$ or $\tilde q$ diverges while $z\,\tilde p$ and $z^2\,\tilde q$ remain finite at $z=0$; and it is an irregular singular point if $z\,\tilde p$ or $z^2\,\tilde q$ diverges at $z=0$.

It is worthwhile pausing here to check the singularity structure in a couple of examples. Consider first the associated Legendre equation (2.28). Rewriting the equation in the form (4.1), we have

$$y''-\frac{2x}{1-x^2}\,y'+\Big(\frac{\lambda}{1-x^2}-\frac{m^2}{(1-x^2)^2}\Big)\,y=0\,. \tag{4.5}$$

Thus we see that all finite values of x except $x=\pm1$ are ordinary points. There are regular singular points at $x=\pm1$. Defining $x=1/z$, one finds that (4.5) becomes

$$\frac{d^2y}{dz^2}-\frac{2z}{1-z^2}\,\frac{dy}{dz}-\Big(\frac{\lambda}{z^2(1-z^2)}+\frac{m^2}{(1-z^2)^2}\Big)\,y=0\,. \tag{4.6}$$

This shows that $z=0$ is a regular singular point too. Therefore the singularities of the associated Legendre equation comprise three regular singular points, at $x=(-1,1,\infty)$. These are also the singularities in the special case of the Legendre equation, where $m=0$. It is, by the way, no coincidence that the "trouble spots" that we encountered when constructing the series expansion of the Legendre equation were at $x=\pm1$, precisely at the locations of singular points of the equation.

We also encountered Bessel's equation, given by (2.33). Dividing by x^2, this becomes

$$y''+\frac{1}{x}\,y'+\Big(1-\frac{\nu^2}{x^2}\Big)\,y=0\,, \tag{4.7}$$

showing that the only singular point within the range of finite x is a regular singular point at $x=0$. Replacing x by $z=1/x$ to analyse the point at infinity, we find that Bessel's equation becomes

$$\frac{d^2y}{dz^2}+\frac{1}{z}\,\frac{dy}{dz}+\Big(\frac{1}{z^4}-\frac{\nu^2}{z^2}\Big)\,y=0\,. \tag{4.8}$$

The $1/z^4$ pole in $\tilde{q}$ at $z = 0$ shows that the Bessel equation (4.7) has an irregular singular point at $x = \infty$, together with its regular singular point at $x = 0$.

It is worth remarking, for future reference, that although Bessel's equation has an irregular singular point, it is one of a rather specific kind, with a $1/z^4$ pole in the coefficient of y. This can actually be viewed as the superposition or *confluence* of two regular singular points. Consider the situation of an ODE with two regular singular points, at $x = a$ and $x = b$, for example with

$$y'' + p(x)\, y' + \frac{1}{(x-a)^2\,(x-b)^2}\, y = 0\,. \tag{4.9}$$

Let us, for simplicity, suppose that here $p(x)$ has no poles at $x = a$ or $x = b$. Clearly, if we now choose the parameters a and b to be equal then instead of having two regular singular points at $x = a$ and $x = b$, we will have one irregular singular point at $x = a = b$, with a fourth-order pole. Thus we may consider Bessel's equation to be a confluent limit of an equation with three regular singular points. In fact most of the common second-order ODE's that one encounters in physics either directly have three regular singular points, or else they are confluent limits of equations with three regular singular points. So important are such equations that the entire class of second-order ODE's with three regular singular points has been classified, and its solutions studied in great detail. It turns out that by making appropriate transformations of the independent and dependent variables, one can put any such equation into a standard canonical form, which is known as the *Hypergeometric Equation.* In this form, the three regular singular points are located at $x = 0$, $x = 1$ and $x = \infty$. The hypergeometric equation is the following

$$x(x-1)\, y'' + [(a+b+1)\, x - c]\, y' + a\, b\, y = 0\,, \tag{4.10}$$

where a, b and c are constants. The regular singular points at $x = 0$ and $x = 1$ are evident by inspection, and the regular singular point at $x = \infty$ can be seen easily after making the standard $x = 1/z$ transformation.

4.2 The Wronskian

Here, we shall undertake a somewhat more systematic study of some of the properties of second-order ODE's, and their solutions. We shall, as usual, take the equation to be

$$L(y) \equiv y''(x) + p(x)\, y'(x) + q(x)\, y(x) = 0\,. \tag{4.11}$$

To begin, let us consider the question of *how many* independent solutions to this equation there will be.

4.2.1 The Wronskian, and linear independence of solutions

The Wronskian is a function defined as follows. Suppose that y_1 and y_2 are two solutions of (4.11). Then we define the Wronskian $\Delta(y_1, y_2)$ of the two solutions by

$$\Delta(y_1, y_2) \equiv y_1\, y_2' - y_2\, y_1' \,. \tag{4.12}$$

It is evident that if the Wronskian vanishes, then we will have

$$\frac{y_1'}{y_1} = \frac{y_2'}{y_2}\,, \tag{4.13}$$

which integrates to give $\log y_1 = \log y_2 +$ constant, hence implying that $y_1 = c\, y_2$, where c is some constant. Thus the solutions y_1 and y_2 are linearly dependent. Recall that in general a set of functions u_i are said to be linearly dependent if and only if there exists a set of constants a_i, not all zero, such that

$$\sum_i a_i\, u_i = 0\,. \tag{4.14}$$

Conversely, if y_1 and y_2 are linearly dependent, say $y_1 = c\, y_2$, then it follows that the Wronskian vanishes,

$$\Delta(y_1, y_2) = y_1(x)\,(c\, y_1'(x)) - (c\, y_1(x))\, y_1'(x) = 0\,. \tag{4.15}$$

Thus combining this with the previous observation, we have the result that that *the Wronskian $\Delta(y_1, y_2)$ vanishes if and only if the two solutions y_1 and y_2 are linearly dependent.*

In fact, if one is given a particular solution y_1 to the second-order linear ODE, the Wronskian can be used in order to construct a second, linearly-independent solution y_2, as follows.

Let us suppose we are given a solution $y_1(x)$. We then pick a specific point $x = x_0$, which we will view as our starting point. The point x_0 will be assumed to be *generic*, in the sense that $y_1(x_0)$ and $y_1'(x_0)$ are non-vanishing. (If this is not true at a particular point, then we can always move to a nearby point where it will be true.) We may then consider a second solution $y_2(x)$, which we shall characterise by specifying the values of $y_2(x)$ and $y_2'(x)$ at $x = x_0$. These two constants can conveniently be written as

$$y_2(x_0) = \alpha\, y_1(x_0)\,, \qquad y_2'(x_0) = \beta\, y_1'(x_0)\,, \tag{4.16}$$

where α and β are constants. (This is nothing but a specification of the "initial conditions" for $y_2(x_0)$ and $y_2'(x_0)$. It happens to be convenient to express them as constant multiples α and β of the non-vanishing constants $y_1(x_0)$ and $y_1'(x_0)$.) Thus at $x = x_0$, we will have

$$\Delta(y_1, y_2)(x_0) = (\beta - \alpha)\, y_1(x_0)\, y_1'(x_0)\,. \tag{4.17}$$

It is clear therefore that at $x = x_0$, y_2 is linearly independent of y_1 provided that $\beta \neq \alpha$. We now look at what happens to $\Delta(y_1, y_2)$ as we move away from $x = x_0$. To do this, differentiate the definition (4.12) of the Wronskian, and then use the original differential equation (4.11) to simply the result:

$$\begin{aligned}
\frac{d\Delta}{dx} &= y_1\, y_2'' - y_2\, y_1'' \,, \\
&= -y_1\,(p\, y_2' + q\, y_2) + y_2\,(p\, y_1' + q\, y_1)\,, \\
&= -p\,\Delta = -\Delta\, \frac{d\log f}{dx}\,,
\end{aligned} \tag{4.18}$$

where we have defined f, for convenience, by

$$f(x) \equiv \exp\Big(\int_{x_0}^x p(t)\, dt\Big)\,. \tag{4.19}$$

Thus we can integrate (4.18), to give

$$\Delta(x) = \Delta(x_0)\, \exp\Big(-\int_{x_0}^x p(t)\, dt\Big) = \frac{\Delta(x_0)}{f(x)}\,. \tag{4.20}$$

Thus we see that $\Delta(x)$, which was already determined to be non-vanishing at $x = x_0$, will be non-vanishing for all x, at least within some neighbourhood of the point x_0, and hence the solution y_2 is independent of y_1 for all x.

We have established that if we have two solutions y_1 and y_2 for which $y_2'(x_0)/y_2(x_0) \neq y_1'(x_0)/y_1(x_0)$, then these two solutions are linearly independent. In fact we can do better, and actually *construct* such a second independent solution $y_2(x)$, from a given solution $y_1(x)$. To do this, we observe that from the definition of the Wronskian we may deduce

$$\Delta(x) = y_1\, y_2' - y_2\, y_1' = y_1^2\, \frac{d}{dx}\Big(\frac{y_2}{y_1}\Big)\,, \tag{4.21}$$

whence[7]

$$y_2(x) = y_1(x) \int_{x_1}^x \frac{\Delta(t)}{y_1^2(t)}\, dt = \Delta(x_0)\, y_1(x) \int_{x_1}^x \frac{dt}{f(t)\, y_1^2(t)}\,, \tag{4.22}$$

[7]Note that if we have an equation $dF(x)/dx = G(x)$, then when we write down the indefinite integral we write

$$F(x) = \int^x G(t)\, dt\,,$$

taking care to use a symbol for the integration variable that is *not* the same as the variable x. It doesn't matter whether we call it t, or x', or $\tilde{x}$, or y or Ξ; anything but x will do! In some textbooks immense confusion is caused by writing $F(x) = \int^x G(x)\, dx$. The meaning of the variable x that is the argument of $F(x)$, and the variable t that is the (dummy) integration variable, are quite distinct, and different symbols should be used for the two.

where x_1 is an arbitrary constant, and for the second equality we have made use of the expression (4.20). Different choices for x_1 shift the value of the integral by a constant, and therefore shift the expression for for $y_2(x)$ by a constant multiple of $y_1(x)$. This arbitrariness is not of interest to us right now, since we can always take linear superpositions of solutions of a linear equation, and thereby get another solution. Since we already know that $y_1(x)$ solves the equation, it is not interesting, for now, to add a constant multiple of $y_1(x)$ to our construction of a linearly-independent solution y_2. (If $y_2(x)$ is linearly independent of $y_1(x)$, then so is $y_2(x) + k\,y_1(x)$, for any constant k.)

We are also not interested, for now, in the freedom to rescale our second solution $y_2(x)$ by a constant factor; obviously, since the differential equation is linear, then if $y_2(x)$ is a solution then so is $c\,y_2(x)$, for any constant c. We may therefore omit the constant prefactor in (4.22), and work with a rescaled y_2. In summary, we may conclude that if y_1 is a solution of the differential equation (4.11), then a second, linearly independent, solution $y_2(x)$ is given by

$$y_2(x) = \int^x \frac{dt}{y_1^2(t)\, f(t)}\,, \tag{4.23}$$

where $f(t)$ is given by (4.19) and the choice of lower limit of integration is not particularly important. Although it is merely a consistency check that we made no mistakes, it is in fact easy to verify by direct substitution that (4.23) satisfies the original equation (4.11), given that y_1 does.

The question now arises as to whether there could be a third solution y_3 of (4.11), independent both of y_1 and y_2. Our results above would already suggest not, since we followed a rather general route by means of which we were led to construct y_2 in (4.22); the only arbitrariness was in the choice of two constants of integration, and changing these merely rescales our y_2 by a constant factor, and adds a constant multiple of y_1 to it. It is instructive, however, to consider the following direct demonstration that there can be no third independent solution:

Suppose we do postulate a third solution y_3. Our aim will be to show that it can in fact be written as a linear combination of y_1 and y_2. Begin by picking a generic point $x = x_0$, at which we shall specify the values of $y_3(x_0)$ and $y_3'(x_0)$. Rather than saying

$$y_3(x_0) = a\,, \qquad y_3'(x_0) = b\,, \tag{4.24}$$

it is convenient instead to parameterise $y_3(x_0)$ and $y_3'(x_0)$ in terms of constants A and B such that

$$y_3(x_0) = A\,y_1(x_0) + B\,y_2(x_0)\,, \qquad y_3'(x_0) = A\,y_1'(x_0) + B\,y_2'(x_0)\,. \tag{4.25}$$

It is easy to see that this is an equally good parameterisation. Simple algebra shows that the constants A and B are related to a and b by

$$A = \frac{a\, y_2'(x_0) - b\, y_2(x_0)}{\Delta(y_1, y_2)(x_0)}\,, \qquad B = \frac{b\, y_1(x_0) - a\, y_1'(x_0)}{\Delta(y_1, y_2)(x_0)}\,, \tag{4.26}$$

where $\Delta(y_1, y_2)(x_0)$ means the Wronskian evaluated at $x = x_0$, namely

$$\Delta(y_1, y_2)(x_0) = y_1(x_0)\, y_2'(x_0) - y_2(x_0)\, y_1'(x_0)\,. \tag{4.27}$$

The crucial point is that by our intial assumption of the linear independence of y_1 and y_2, we must have $\Delta(y_1, y_2)(x_0) \neq 0$, and thus nothing prevents us solving (4.26) for A and B; we have two independent equations determining the two constants A and B. Now, we can use the original differential equation (4.11) to deduce that

$$\begin{aligned} y_3''(x_0) &= -p(x_0)\, y_3'(x_0) - q(x_0)\, y_3(x_0)\,, && (4.28)\\ &= -p(x_0)\, [A\, y_1'(x_0) + B\, y_2'(x_0)] - q(x_0)\, [A\, y_1(x_0) + B\, y_2(x_0)]\,, && (4.29)\\ &= A\, y_1''(x_0) + B\, y_2''(x_0)\,. \end{aligned}$$

We can then repeat these steps for all the higher derivatives of y_3 at $x = x_0$, deducing that

$$y_3^{(n)}(x_0) = A\, y_1^{(n)}(x_0) + B\, y_2^{(n)}(x_0)\,, \tag{4.30}$$

where $y^{(n)}$ denotes the n'th derivative. But we know from Taylor's theorem that within its radius of convergence, we can write any function $h(x)$ in terms of all its derivatives at $x = x_0$:

$$h(x) = \sum_{n\ge 0} \tfrac{1}{n!}\, (x - x_0)^n\, h^{(n)}(x_0)\,. \tag{4.31}$$

Therefore it follows from (4.30) that

$$\begin{aligned} y_3(x) &= \sum_{n\ge 0} \frac{1}{n!}\, (x - x_0)^n\, y_3^{(n)}(x_0) = \sum_{n\ge 0} \frac{1}{n!}\, (x - x_0)^n\, [A\, y_1^{(n)}(x_0) + B\, y_2^{(n)}(x_0)]\,,\\ &= A\, y_1(x) + B\, y_2(x)\,, && (4.32) \end{aligned}$$

and hence the solution y_3 is linearly dependent on y_1 and y_2, at least within the radius of convergence of the power series expansion around x_0.

To recapitulate, what we did was to consider a completely arbitrary solution y_3 of the second-order ODE (4.11). We showed that it can always be written as a linear combination of the two independent solutions y_1 and y_2, at least within the range of x for which they have convergent power-series expansions. Therefore there are exactly two linearly independent solutions. It is clear that very similar arguments could be used for an N'th-order ODE, and would show that it has N linearly-independent solutions.

4.3 Solution of the inhomogeneous equation

We have so far considered the solutions of the homogeneous equation (4.11), or $L(y) = 0$, for which each term is of degree 1 in y or its derivatives. We may also consider the *inhomogeneous* equation $L(y) = r(x)$, i.e.

$$L(y) \equiv y''(x) + p(x)\, y'(x) + q(x)\, y(x) = r(x)\,. \tag{4.33}$$

One can think of the function $r(x)$ as being like a "source term" for the field y. Here, we shall show that we can obtain a formal solution for this equation, in terms of the two linearly-independent solutions y_1 and y_2 of the homogeneous equation, $L(y_1) = 0$, $L(y_2) = 0$ that we discussed previously. In other words, we suppose that we know how to solve the homogeneous equation, and now we wish to use these known solutions y_1 and y_2 in order to obtain the solution of the inhomogeneous equation.

To do this, first consider what happens if we write $y = u\, v$ in (4.33). It follows that

$$\begin{aligned} L(u\,v) &= (u\,v)'' + p\,(u\,v)' + q\,u\,v\,, \\ &= v\,u'' + v\,p\,u' + v\,q\,u + u\,v'' + p\,u\,v' + 2u'\,v'\,, \\ &= v\,L(u) + u\,v'' + (u\,p + 2u')\,v' = r\,. \end{aligned} \tag{4.34}$$

Now choose $u = y_1$, where y_1 is one of the solutions of the homogeneous equation, $L(y_1) = 0$. Thus we get

$$v'' + \Big(p + 2(y_1'/y_1)\Big)\, v' = r/y_1\,, \tag{4.35}$$

after dividing out by y_1. Our task is to solve for v. We saw previously from the definition (4.12) of the Wronskian that $(y_2/y_1)' = \Delta/y_1^2$, and also $\Delta' = -p(x)\,\Delta$, and hence we will have

$$\Big(\frac{y_2}{y_1}\Big)'' = \Big(\frac{\Delta}{y_1^2}\Big)' = \frac{\Delta'}{y_1^2} - 2\,\frac{y_1'\,\Delta}{y_1^3} = -p\,\frac{\Delta}{y_1^2} - 2\,\frac{y_1'}{y_1}\,\frac{\Delta}{y_1^2} = -(p + 2(y_1'/y_1))\,\frac{\Delta}{y_1^2}\,. \tag{4.36}$$

This can therefore be written as

$$(y_2/y_1)'' + [p + 2(y_1'/y_1)]\,(y_2/y_1)' = 0\,. \tag{4.37}$$

Next, multiply this equation by v', multiply (4.35) by $(y_2/y_1)'$, and subtract the former from the latter. This gives

$$v''\,(y_2/y_1)' - v'\,(y_2/y_1)'' = (r/y_1)\,(y_2/y_1)'\,, \tag{4.38}$$

which can be rewritten as

$$[(y_2/y_1)']^2\,\frac{d}{dx}\Big(\frac{v'}{(y_2/y_1)'}\Big) = (r/y_1)\,(y_2/y_1)'\,, \tag{4.39}$$

and hence

$$\frac{d}{dx}\Big(\frac{v'}{(y_2/y_1)'}\Big) = \frac{r\,y_1}{\Delta}\,. \tag{4.40}$$

This equation can be integrated once to give

$$v' = (y_2/y_1)' \int \frac{r\,y_1}{\Delta}\,, \tag{4.41}$$

or, in other words,

$$v' = -\frac{r\,y_2}{\Delta} + \frac{d}{dx}\Big[(y_2/y_1) \int \frac{r\,y_1}{\Delta}\Big]\,. \tag{4.42}$$

Integrating again, we have

$$v = -\int \frac{r\,y_2}{\Delta} + \frac{y_2}{y_1} \int \frac{r\,y_1}{\Delta}\,. \tag{4.43}$$

Now recall that we originally expressed our solution y of the inhomogeneous equation $L(y) = r$ as $y = y_1\,v$. Therefore, we have the formal result that y is given by

$$y = -y_1 \int \frac{r y_2}{\Delta} + y_2 \int \frac{r\,y_1}{\Delta}\,. \tag{4.44}$$

Making this more explicit, it reads

$$y(x) = y_2(x) \int^x dt\, \frac{r(t)\,y_1(t)}{y_1(t)\,y_2'(t) - y_2(t)\,y_1'(t)} - y_1(x) \int^x dt\, \frac{r(t)\,y_2(t)}{y_1(t)\,y_2'(t) - y_2(t)\,y_1'(t)}\,. \tag{4.45}$$

Thus we have the answer expressed purely in terms of the two independent solutions y_1 and y_2 of the homogeneous equation (which we suppose we know), and the source term r in (4.33). Note that what we have written in (4.45) is a particular solution, to which arbitrary amounts of the two homogeneous solutions y_1 and y_2 can be added. In fact the freedom to change the lower limits of integration in the two integrals in (4.45) precisely corresponds to adding multiples of the solutions $y_1(x)$ and $y_2(x)$ of the homogeneous equation.

4.4 Series solutions of the homogeneous equation

4.4.1 Expansion around ordinary point

Let us now return to a more detailed study the construction of series solutions of second-order linear ODE's. To begin, consider the case where we expand the solution of (4.11) around an ordinary point $x = a$, i.e. a point for which $p(a)$ and $q(a)$ are finite. More precisely, we require thta $p(x)$ and $(q(x)$ are analytic at $x = a$, which means that in the vicinity of $x = a$, we can expand them in Taylor series:

$$\begin{aligned} p(x) &= p(a) + (x-a)\,p'(a) + \tfrac{1}{2}(x-a)^2\,p''(a) + \cdots\,, \\ q(x) &= q(a) + (x-a)\,q'(a) + \tfrac{1}{2}(x-a)^2\,q''(a) + \cdots\,. \end{aligned} \tag{4.46}$$

Let us try assuming that the solution $y(x)$ is also analytic near $x=a$, so we can also expand it in a Taylor series:

$$y(x)=\sum_{n\ge 0} a_n\,(x-a)^n = a_0 + a_1\,(x-a) + a_2\,(x-a)^2 + \cdots\,. \tag{4.47}$$

Substituting these into (4.11), we get

$$\begin{aligned} 0 &= [2a_2 + a_1\,p(a) + a_0\,q(a)] \\ &\quad +[6a_3 + 2a_2\,p(a) + a_1\,p'(a) + a_0\,q'(a) + a_1\,q(a)]\,(x-a) + \cdots\,. \end{aligned} \tag{4.48}$$

By equating the coefficients of each power of $(x-a)$ to zero, we obtain a sequence of equations that determine the coefficients a_n with $n\ge 2$ in terms of a_0 and a_1. Thus from the first term, in $(x-a)^0$, we solve for a_2 in terms of a_0 and a_1,

$$a_2 = -\tfrac12(a_1\,p(a) + a_0\,q(a))\,. \tag{4.49}$$

From the term in $(x-a)^1$, we then solve for a_3 in terms of a_0, a_1 and a_2. Since we have already solved for a_2 in terms of a_0 and a_1, this then gives us a_3 in terms of a_0 and a_1. Continuing to higher orders, we thus obtain all the a_n for $n\ge 2$ in terms of a_0 and a_1.

Since the two initial coefficients a_0 and a_1 are arbitrary, these parameterise the two-dimensional space of solutions of the second-order ODE. Thus we may think of the general solution as being given by

$$y = a_0\,y_1 + a_1\,y_2\,, \tag{4.50}$$

where y_1 and y_2 are the two independent solutions determined by our series expansions. (The solution y_1 is the one obtained by taking $a_1=0$, while the solution y_2 is obtained by taking $a_0=0$.) Solving for the various higher coefficients a_n as described above, one finds that the two solutions are given by

$$\begin{aligned} y_1 &= 1 - \tfrac12 q(a)\,(x-a)^2 + \tfrac16[(q(a)p(a) - q'(a)]\,(x-a)^3 + \cdots\,, \\ y_2 &= (x-a) - \tfrac12 p(a)\,(x-a)^2 + \tfrac16[p^2(a) - p'(a) - q(a)]\,(x-a)^3 + \cdots\,. \end{aligned} \tag{4.51}$$

Note that the two basic solutions y_1 and y_2 have the convenient properties that

$$\begin{aligned} y_1(a) &= 1\,, \qquad y_1'(a) = 0\,, \\ y_2(a) &= 0\,, \qquad y_2'(a) = 1\,. \end{aligned} \tag{4.52}$$

Thus if one is looking for the solution that satisfies the boundary conditions $y(a)=A$, $y'(a)=B$, then the answer is $y = A\,y_1 + B\,y_2$.

We were able to obtain analytic solutions (i.e. solutions as Taylor series) in the neighbourhood of $x = a$ because this was an ordinary point, where $p(x)$ and $q(x)$ were finite, and themselves had Taylor-series expansions. The series solution will be valid within a radius of convergence determined by the closest singular point. Thus, for example, if there is a singular point of the ODE at $x = b$, where $b > a$, then the series solutions will converge for all x such that

$$|x - a| < b - a\,. \tag{4.53}$$

In general, the series solutions will become divergent when x approaches either of the values that saturates this inequality. We saw an example of this when we studied the series solution of the Legendre equation. We expanded around the ordinary point at $x = 0$, and sure enough, we found that the series solutions became divergent at $x = \pm 1$, which correspond to regular singular points of the Legendre equation. (Of course we also observed that in that case we could arrange, by a judicious choice of the parameters of the equation, to get a power-series solution that actually terminated, thereby avoiding the divergence of the generic solution.)

4.4.2 Expansion around singular point

So far, we considered the case where we expand around an ordinary point $x = a$, for which $p(a)$ and $q(a)$ are analytic at $x = a$. Suppose now that the function $p(x)$ has a pole at $x = a$, while $q(x)$ is still analytic. Let us assume that $p(x)$ has a pole of degree N, which means that is has an expansion of the form

$$p(x) = \sum_{k=-N}^{\infty} a_k\,(x - a)^k\,. \tag{4.54}$$

A convenient way to write this is as

$$p(x) = \frac{F(x)}{(x - a)^N}\,, \tag{4.55}$$

where $F(x)$ is analytic at $x = a$, implying that it has a Taylor expansion

$$F(x) = F(a) + F'(a)\,(x - a) + \tfrac{1}{2!}\,F''(a)\,(x - a)^2 + \cdots\,, \tag{4.56}$$

and hence

$$p(x) = \frac{F(a)}{(x - a)^N} + \frac{F'(a)}{(x - a)^{N-1}} + \frac{F''(a)}{2(x - a)^{N-3}} + \cdots\,. \tag{4.57}$$

Note that $F(a)$ must be nonzero, since we are assuming that the coefficient of the leading-order $(x - a)^{-N}$ pole is nonzero. As we shall illustrate below, we will now find that certain of the coefficients a_i in the series expansion (4.47) are zero, namely

$$a_1 = a_2 = \cdots = a_N = 0\,. \tag{4.58}$$

However, the coefficients a_{N+1}, a_{N+2}, $a_{N+3}, \cdots$ can be solved for in terms of a_0. This means that in this case we have found just one of the two independent solutions of the ODE as a series expansion of the form (4.47).

Here's an example to show what is happening. Suppose that $p(x)$ has a double pole at $x = a$ (i.e. $N = 2$). Thus we have

$$p(x) = \frac{F(x)}{(x-a)^2}\,. \tag{4.59}$$

Plugging the series expansion (4.47) into the equation (4.11), with this assumed form for $p(x)$, we will get

$$\begin{aligned} 0 &= \frac{a_1\,F(a)}{(x-a)^2} + \frac{2a_2\,F(a) + a_1\,F'(a)}{x-a} \\ &\quad + [2a_2 + q(a)\,a_0 + 3a_3\,F(a) + 2a_2\,F'(a) + \tfrac{1}{2}a_1\,F''(a)] + \cdots\,. \end{aligned} \tag{4.60}$$

Thus the coefficient of $(x-a)^{-2}$ tells us that $a_1 = 0$ (recall that $F(a) \ne 0$, which in turn means that the coefficient of $(x-a)^{-1}$ implies that $a_2 = 0$. The coefficient of $(x-a)^0$ then allows us to solve for a_3 in terms of a_0. The higher powers of $(x-a)$ will then allow us to solve for a_4, a_5, *etc.*, in terms of a_0. It is not hard to see that this gives the series solution

$$y_1 = 1 - \frac{q(a)}{3F(a)}\,(x-a)^3 + \Big[\frac{q(a)}{2F^2(a)} + \frac{q(a)\,F'(a)}{4F^2(a)} - \frac{q'(a)}{4F(a)}\Big]\,(x-a)^4 + \cdots\,, \tag{4.61}$$

where we have, for simplicity, taken $a_0 = 1$.

We've found one solution in this example, as a power series in $(x-a)$. But what of the other solution? We know from our previous general analysis that there should be two independent solutions. Evidently, the second solution must not be expressible as a power series of the form (4.47); hence our failure to find it by this means. Recall, however, that we were able earlier to give a general construction of the second, linearly-independent, solution of any second-order ODE, if we were given one solution. The second solution was given by (4.22), and thus is of the form

$$y_2(x) = y_1(x)\int^x \frac{dt}{f(t)\,y_1^2(t)}\,, \tag{4.62}$$

where $p(x) = d\log f/dx$. Now, we are assuming that $p(x)$ is given by (4.59), where $F(x)$ is analytic at $x = a$ (i.e. it admits a Taylor expansion around the point $x = a$). Therefore we can expand $F(x)$ in a power series, giving

$$p(x) = \frac{F(a)}{(x-a)^2} + \frac{F'(a)}{x-a} + \frac{1}{2}F''(a) + \tfrac{1}{6}F'''(a)\,(x-a) + \cdots\,. \tag{4.63}$$

Thus we have

$$\log f = \int^x p = -\frac{F(a)}{x-a} + F'(a)\,\log(x-a) + \tfrac{1}{2}F''(a)\,(x-a) + \cdots\,, \tag{4.64}$$

whence

$$\begin{aligned}\frac{1}{f(x)} &= \exp\Big(\frac{F(a)}{x-a}\Big)\,(x-a)^{-F'(a)}\,\exp[-\tfrac{1}{2}F''(a)\,(x-a)+\cdots]\,,\\ &= \exp\Big(\frac{F(a)}{x-a}\Big)\,(x-a)^{-F'(a)}\,G(x)\,,\end{aligned} \tag{4.65}$$

where $G(x)$ is an analytic function. Since $y_1(x)$ is an analytic function (admiting a Talor expansion around the point $x = a$), it follows that $1/y_1^2(x)$ is analytic too, and so finally we conclude from (4.62) that

$$y_2(x) = y_1(x)\int^x e^{F(a)/(t-a)}\,(t-a)^{-F'(a)}\,H(t)\,dt\,, \tag{4.66}$$

where $H(t) = G(t)/y_1^2(t)$ is some analytic function.

The function (4.66) behaves badly at $t = a$, because of the factor $e^{F(a)/(t-a)}$. For example, if $F(a)$ is positive, this function blows up faster than *any* power of $(t-a)$ as t approaches a from above. (Think of the power-series expansion for e^z to see this; $e^z = \sum_{n\ge0} z^n/n!$. If z is big enough, then the higher and higher powers of z become the dominant ones here.) Such divergent behaviour which is worse than any power law is known as an *essential singularity.* Functions with this type of behaviour cannot be expanded in a Taylor series around the essential singularity. This explains why we were unable to find a power-series expansion for the second solution in this case.

We ran into this problem with the construction of the second solution because we assumed that $p(x)$ had a double pole at $x = a$, as in (4.59). Suppose instead $p(x)$ had only a single pole, so that

$$p(x) = \frac{F(x)}{x-a}\,, \tag{4.67}$$

where $F(x)$ is analytic at $x = a$. Thus we will now have

$$p(x) = \frac{F(a)}{x-a} + F'(a) + \tfrac{1}{2}F''(a)\,(x-a) + \cdots\,. \tag{4.68}$$

Integrating to get $\log f$, we will now have

$$\log f = F(a)\,\log(x-a) + F'(a)\,(x-a) + \cdots\,, \tag{4.69}$$

and so (4.62) will now give

$$y_2(x) = y_1(x)\int^x (t-a)^{-F(a)}\,H(t)\,dt\,, \tag{4.70}$$

where $H(t)$ is some analytic function. This is a much better situation than the previous one. Now, instead of an essential singularity, we instead merely face a power-law singular behaviour. In fact if we expand $H(t)$ in a Taylor series around $t = a$,

$$H(t) = \sum_{n\geq 0} h_n\,(t-a)^n\,, \tag{4.71}$$

we can integrate term by term in (4.70), leading to a result of the form

$$y_2(x) = y_1(x)\,\sum_{n\geq 0} c_n\,(x-a)^{n+1-F(a)}\,. \tag{4.72}$$

(We shall assume, for now, that $F(a)$ is not an integer.) The series therefore involves fractional powers of $(x-a)$. This is a rather mild kind of singularity, called a *branch cut*. We will study such things in more detail later in the course.

Let us pause to summarise what we have discovered. If we look at an ordinary point $x = a$, for which $p(a)$ and $q(a)$ are finite, then we can obtain the two independent solutions of the second-order ODE (4.11) as power-series expansions of the form (4.47). If, on the other hand, $p(x)$ has a pole at $x = a$, while $q(a)$ is still assumed to be finite, then we can only obtain one solution of the ODE as a power series of the form (4.47). The second solution must instead now be obtained using the general construction (4.62). However, if $p(x)$ has a pole of degree $N \geq 2$, the behaviour of this second solution will be very bad around $x = a$, with an essential singularity. By contrast, if $p(x)$ has only a simple pole, the second solution will be much better behaved. It will still, in general, not be a simple power series, but it will have nothing worse than a branch-cut singularity in its behaviour around $x = a$. In fact, it is evident from (4.72) that the second solution, in the case where $p(x)$ has a pole only of degree $N = 1$, has a series expansion of the form

$$y_2(x) = \sum_{n\geq 0} b_n\,x^{n+s}\,, \tag{4.73}$$

for some coefficients b_n, where s is a constant related to $F(a)$.

In general, we can define a *Regular Singular Point* as one where the general solution of the ODE has a pole or branch cut. On the other hand, an *Irregular Singular Point* is defined to be one where the general solution has an essential singularity.

4.4.3 Indicial Equation

We analysed above what happens if $q(x)$ is analytic at $x = a$, but $p(x)$ is singular. Suppose now that we consider the more general situation where both $p(x)$ and $q(x)$ are singular at

$x = a$. Specifically, let us consider the situation when

$$p(x) = \frac{F(x)}{(x-a)^N}\,, \qquad q(x) = \frac{G(x)}{(x-a)^M}\,, \tag{4.74}$$

where $F(x)$ and $G(x)$ are themselves analytic at $x = a$, and N and M are positive integers.

To study the behaviour of the solutions, let us consider a solution y of $L(y) = 0$, where we shall write $y = u\,v$. The idea is that we are going to factor off all the singular behaviour of y in the function v, while u will be taken to be analytic. (Clearly we can always make some such split; if all else failed, we could take $u = 1$, after all! The key point is that we want to make a *useful* split of this sort). Now, it follows that our equation $L(y) = y'' + p\,y' + q\,y = 0$ becomes

$$u'' + H\,u' + J\,u = 0\,, \tag{4.75}$$

where the functions H and J are given by

$$H = p + \frac{2v'}{v}\,, \qquad J = q + \frac{v''}{v} + \frac{p\,v'}{v}\,. \tag{4.76}$$

Now, from what we saw in the previous section, we know that provided the function J in (4.75) is analytic, there will be at least one analytic solution u, even if H has a pole. Thus we will consider cases where H has poles, but where we can *choose* the function v in such a way that J is analytic. We shall then choose u to be the analytic solution of (4.75).

Let us suppose that $x = a$ is a regular singular point. This corresponds to the case where $p(x)$ has a pole of order 1, and $q(x)$ has a pole of order 2. From the previous discussion, we are expecting that the solution will have singular behaviour of the general form $(x - a)^s$. In fact, to begin with let us try taking the function v, into which we are factoring off the singular behaviour, to be given precisely by

$$v = (x-a)^s\,, \tag{4.77}$$

for some constant index s. This implies that $v'/v = s/(x-a)$ and $v''/v = s(s-1)/(x-a)^2$, and hence J defined in (4.76) is given by

$$J = q(x) + \frac{s\,p(x)}{x-a} + \frac{s(s-1)}{(x-a)^2}\,. \tag{4.78}$$

With $p(x)$ having a first-order pole, and $q(x)$ a second-order pole, we can write

$$p(x) = \frac{F(x)}{x-a}\,, \qquad q(x) = \frac{G(x)}{(x-a)^2}\,, \tag{4.79}$$

where $F(x)$ and $G(x)$ are analytic. Thus we have

$$p(x) = \frac{F(a)}{x-a} + F'(a)\cdots\,, \qquad q(x) = \frac{G(a)}{(x-a)^2} + \frac{G'(a)}{x-a} + \cdots\,, \tag{4.80}$$

and so

$$J = \frac{G(a) + s\,F(a) + s\,(s-1)}{(x-a)^2} + \frac{G'(a) + s\,F'(a)}{x-a} + \text{regular terms}\,. \tag{4.81}$$

Assume for a moment that $G'(a) + s\,F'(a) = 0$, so that there is no $1/(x-a)$ term. We see that we can then make J completely regular if we choose s such that the coefficient of $1/(x-a)^2$ vanishes. This is achieved if s satisfies the so-called *Indicial Equation*

$$s^2 + [F(a) - 1]\,s + G(a) = 0\,. \tag{4.82}$$

Its two roots, which we may call s_1 and s_2, correspondingly give us two solutions of the original ODE,

$$y_1 = (x-a)^{s_1}\,u_1\,, \qquad y_2 = (x-a)^{s_2}\,u_2\,, \tag{4.83}$$

where u_1 and u_2 are analytic at $x = a$. Without loss of generality, it is useful to assume that we order the roots so that

$$s_1 \ge s_2\,. \tag{4.84}$$

Now suppose that $G'(a) + s\,F'(a)$ is non-zero, which means we also have a $1/(x-a)$ singular term in J. To handle this, we just have to modify slightly our choice of how to factor off the singular behaviour of the solution when we write $y(x) = u(x)\,v(x)$. We do this by choosing

$$v(x) = (x-a)^s\,e^{\beta\,x}\,. \tag{4.85}$$

A straightforward calculation using (4.78) now shows that we shall have

$$J = \frac{G(a) + s\,F(a) + s\,(s-1)}{(x-a)^2} + + \frac{G'(a) + s\,F'(a) + 2s\,\beta + \beta\,F(a)}{x-a} + \text{regular terms}\,. \tag{4.86}$$

The condition for removing the $1/(x-a)^2$ singularity is unchanged from before; we should take s to satisfy the indicial equation (4.82). We now use the additional freedom associated with the introduction of the constant β, which we choose such that the coefficient of $1/(x-a)$ vanishes also. Having thus arranged that J is analytic, we therefore again know that we can find at least one analytic solution $u(x)$ to the equation (4.75), and thus we will get a solution to the original differential equation of the form $y(x) = u(x)\,(x-a)^s\,e^{\beta\,x}$. Since $e^{\beta\,x}$ is analytic, we again have the conclusion that $y(x)$ is expressed as $(x-a)^s$ times an analytic function, where s is determined by the indicial equation (4.82).

In a generic case where the two roots s_1 and s_2 satisfy $s_1 - s_2 \ne$ integer, we obtain two independent solutions by this method. If, on the other hand, $s_1 = s_2$, (and usually, if $s_1 - s_2$ =integer), one finds that u_2 is related to u_1 by $u_2 = (x-a)^{s_1 - s_2}\,u_1$, and so from

(4.83) we see that we will get only one solution by this method. The second solution can, however, still be obtained using (4.22),

$$y_2(x) = y_1(x) \int^x \frac{dt}{f(t)\, y_1(t)^2}\,, \tag{4.87}$$

where A is a constant, and $p(x)$ is written as $p = d\log f/dx$. Let us look at this in more detail.

Since $p(x)$ is given by (4.79) it follows that

$$\frac{1}{f(x)} = \exp\Big(-\int^x \frac{F(a)}{(t-a)}\, dt + \cdots\Big) = (x-a)^{-F(a)}\, g(x)\,, \tag{4.88}$$

where $g(x)$ is the analytic function that comes from integrating the higher-order terms. Now, the indicial equation (4.82) can be written as $(s-s_1)(s-s_2)=0$, where s_1 and s_2 are its roots, and so we see that $s_1+s_2 = 1-F(a)$, and hence $1/f(x)$ in (4.88) has the form $(x-a)^{1-s_1-s_2}$ times the analytic function $g(x)$. Plugging the form of the first solution given in (4.83), for y_1, into (4.87), we therefore find that the integrand is of the form

$$\frac{(t-a)^{s_1+s_2-1}\, g(t)}{(t-a)^{2s_1}\, u_1(t)^2} = h(t)\,(t-a)^{-s_1+s_2-1}\,, \tag{4.89}$$

where $h(t) = g(t)/u_1(t)^2$ is again analytic. If we expand $h(t)$ as

$$h(t) = \sum_{n\ge 0} b_n\,(t-a)^n\,, \tag{4.90}$$

then inserting this into (4.89), and then (4.87), and integrating term by term, we obtain an expression for the second solution $y_2(x)$. In general, i.e. when s_1-s_2 is not equal to an integer, this will give

$$y_2(x) = u_1(x) \sum_{n\ge 0} \frac{b_n}{n-s_1+s_2}\,(x-a)^{n+s_2}\,. \tag{4.91}$$

If s_1-s_2 is not equal to an integer, we saw previously that we had already found the two linearly-independent solutions of the differential equation, given in (4.83). In these circumstances, the solution (4.91) must be just equivalent to the second solution already found in (4.83).[8]

[8]The expression for $y_2(x)$ in (4.83) and the expression for $y_2(x)$ in (4.91) may not be literally identical; the one may be related to the other by a constant scaling and the addition of some constant multiple of $y_1(x)$. The essential point is that when s_1-s_2 is not an integer, the expression for $y_2(x)$ in (4.83) is *guaranteed* to be linearly independent of $y_1(x)$. Likewise, our construction of a second solution $y_2(x)$ in (4.91) is also *guaranteed* to be linearly independent of $y_1(x)$. It is to be hoped that no undue confusion has been casued by giving the results of these two constructions for the second solution the same name $y_2(x)$.

If instead s_1-s_2 is an integer, it is clear from (4.91) that if the constant b_n with $n = s_1-s_2$ is non-vanishing, then the expression (4.91) is invalid, because of the vanishing denominator $n-s_1+s_2$ for this term in the sum. What has happened, of course, is that this term in (4.91) came from integrating $1/(t-a)$. In the usual way, $\int^x dt\,(t-a)^k = (x-a)^{k+1}/(k+1)$ for all values of the constant k except for $k=-1$, when instead we get $\int^x dt\,(t-a)^{-1} = \log(x-a)$. Thus, when $s_1 - s_2$ is an integer we must omit the term with $n = s_1 - s_2$ from the sum in (4.91), and handle the integration separately. The net result is that we get

$$y_2(x) = b_{s_1-s_2}\, y_1(x)\, \log(x-a) + u_1(x) \sum_{n\ge 0}{}' \frac{b_n}{n-s_1+s_2}\,(x-a)^{n+s_2}\,, \tag{4.92}$$

where we use the notation $\sum'_{n\ge0}$ to indicate that the term $n = s_1 - s_2$ is omitted in the summation. Thus in general, to find the second independent solution in a series expansion around a regular singular point $x = a$, we should include a $\log(x-a)$ term in the postulated form of the second solution. In fact, from (4.92), we see that we should try a series expansion

$$y_2(x) = A\, y_1(x)\, \log(x-a) + \sum_n c_n\,(x-a)^{n+s}\,, \tag{4.93}$$

where A is a constant and $y_1(x)$ is the first solution.

It is becoming clear by this stage that one could spend a lifetime exploring all the special cases and abnormalities and perversities in the structure of the solutions of ODE's. Let us therefore bring this discussion to a close, with a summary of what we have found, and what one finds in a more exhaustive analysis of all the possibilities.

1. If we are seeking series solutions expanded around an *ordinary point* $x = a$ of the differential equation $y'' + p(x)\, y' + q(x)\, y = 0$ (where, by definition, $p(x)$ and $q(x)$ are analytic at $x = a$), then the solutions will both be analytic, and take the form

$$y(x) = \sum_{(n)\ge 0} a_n\,(x-a)^n\,. \tag{4.94}$$

The coefficients a_n satisfy a recursion relation which determines all the a_n in terms of a_0 and a_1. Thus we have two linearly-independent analytic solutions.

2. If we are seeking series solutions expanded around a *regular singular point* $x = a$ of the differential equation $y'' + p(x)\, y' + q(x)\, y = 0$ (where, by definition, $p(x)$ and $q(x)$ are of the forms $p(x) = F(x)/(x-a)$ and $q(x) = G(x)/(g-a)^2$, where $F(x)$ and $G(x)$ are analytic at $x = a$), then we should try an expansion of the form

$$y(x) = \sum_{n\ge 0} a_n\,(x-a)^{n+s}\,. \tag{4.95}$$

The coefficients a_n will satisfy a recursion relation, and in addition the quantity s will satisfy an *indicial equation*, quadratic in s:

$$(s - s_1)(s - s_2) = 0\,. \tag{4.96}$$

If $s_1 - s_2 \neq$ integer, one will obtain the two independent solutions by this method, associated with the two values $s = s_1$ and $s = s_2$ for the index. If $s_1 = s_2$, and usually, if $s_1 - s_2 =$ integer, only one linearly independent solution, say $y_1(x)$, will arise from this construction. The second solution can be obtained by trying a series expansion of the form

$$y_2(x) = A\, y_1(x)\, \log(x - a) + \sum_{n\ge 0} c_n\, (x - a)^n\,. \tag{4.97}$$

3. If $p(x)$ has a pole of order higher than 1 at $x = a$, or $q(x)$ has a pole of order higher than 2 at $x = a$, then at least one, and possibly both, of the solutions will have an essential singularity at $x = a$. Note, however, that if $q(x)$ is analytic while $p(x)$ has a pole of arbitrary order n, then one of the solutions is analytic at $x = a$, as we saw in section 4.4.2.

4. If $p(x)$ or $q(x)$ themselves have worse singularities than poles, the solutions will be even more pathological.

Finally, here is an example of the application of the series solution technique, in the case of the Bessel equation,

$$x^2\, y'' + x\, y' + (x^2 - \nu^2)\, y = 0\,, \tag{4.98}$$

where ν is a constant, given, parameter in the equation. As we have already discussed, this equation has a regular singular point at $x = 0$, and an irregular singular point at $x = \infty$. We shall perform a series expansion around $x = 0$. Since this is a regular singular point, we therefore seek solutions of the form

$$y(x) = \sum_{n\ge 0} a_n\, x^{n+\sigma}\,. \tag{4.99}$$

Substituting into (4.98), we obtain

$$\sum_{n\ge 0} [(n+\sigma)^2 - \nu^2]\, a_n\, x^{n+\sigma} + \sum_{n\ge 0} a_n\, x^{n+\sigma+2} = 0\,. \tag{4.100}$$

Since this must hold for all x, we ca now equate to zero the coefficient of each power of x. To do this, in the first sum we make the replacement $n \to n + 2$, so that (4.100) is re-expressed as[9]

$$\sum_{n\geq 0}\Big\{[(n+\sigma+2)^2-\nu^2]\,a_{n+2}+a_n\Big\}\,x^{n+\sigma+2}+\sigma^2\,a_0\,x^\sigma+(\sigma+1)^2\,a_1\,x^{\sigma+1}=0\,. \tag{4.101}$$

From this we see that

$$a_{n+2}=\frac{a_n}{\nu^2-(n+\sigma+2)^2}\,, \tag{4.102}$$

for $n\geq 0$. In addition we have, from the two "extra" terms,

$$(\sigma^2-\nu^2)\,a_0=0\,,\qquad [(\sigma+1)^2-\nu^2]\,a_1=0\,. \tag{4.103}$$

We begin with the first equation in (4.103). This is the *Indicial Equation.* Notice that we can in general insist, without any loss of generality, that $a_0\neq 0$. The reason for this is as follows. Suppose a_0 *were* equal to zero. The series (4.99) would then begin with the a_1 term, so it would be a series whose powers of x were $(x^{\sigma+1},x^{\sigma+2},x^{\sigma+3},\ldots)$. But since at the stage when we write (4.99) σ is a completely arbitrary constant, not yet determined, we could as well relabel it by writing $\sigma=\sigma'-1$. We would then have a series whose powers of x are $(x^{\sigma'},x^{\sigma'+1},x^{\sigma'+2},\ldots)$. But this is exactly what we would have had if the a_0 term were in fact non-zero, after relabelling σ' as σ. So insisting that a_0 be non-zero loses no generality at all.

Proceeding, we then have the indical equation $\sigma^2-\nu^2=0$, i.e.

$$\sigma=\pm\nu\,. \tag{4.104}$$

Now we look at the second equation in (4.103). Since we already know from the indicial equation that $\sigma^2=\nu^2$, we can rewrite the second equation as

$$(2\sigma+1)\,a_1=0\,. \tag{4.105}$$

Thus either $a_1=0$ or else $\sigma=-\frac{1}{2}$. But since we already know from the indicial equation that $\sigma=\pm\nu$, it follows that except in the very special case where $\nu=\frac{1}{2}$, which has to be analysed separately, we must have that $a_1=0$. Let us assume that $\nu\neq\pm\frac{1}{2}$, for simplicity. In fact, we shall assume for now that ν takes a generic value, which is not equal to any integer or half integer.

[9]Recall that "sending $n\rightarrow n+2$ in the first sum" means first setting $n=m+2$, so that the summation over m runs from -2 up to $+\infty$. Then, we write this as the sum from $m=0$ to $+\infty$ together with the "extra" two terms $m=-2$ and $m=-1$ added on in addition. Finally, we relabel the m summation variable as n.

Finally, in the recursion relation (4.102), we substitute the two possible values for σ, i.e. $\sigma = \nu$ or $\sigma = -\nu$. In each of these two cases, the recursion relation then gives us expressions for all the a_n with $n \ge 2$, in terms of a_0 (which is non-zero), and a_1 (which is zero since we are assuming $\nu \ne \pm\frac{1}{2}$).

We can check the radius of convergence of the series solutions, by applying the ratio test. The ratio of successive terms (bearing in mind that $a_1 = 0$, which means all the odd a_n are zero) is given by

$$\frac{a_{n+2}\, x^2}{a_n} = \frac{x^2}{\nu^2 - (n+\sigma+2)^2}\,, \tag{4.106}$$

where $\sigma = \pm\nu$. In either case, at large n we see that the absolute value of the ratio tends to x^2/n^2, and thus the ratio becomes zero for any fixed x, no matter how large. Thus the radius of convergence is infinite. Notice that this accords perfectly with the fact that the next nearest singular point of the Bessel equation is at $x = \infty$. Thus we should expect the series to converge for any finite x.

We can easily see that with ν taking a generic value (neither integer nor half-integer), our two solutions corresponding to the two roots of the indicial equation $\sigma^2 - \nu^2 = 0$, namely $\sigma = +\nu$ and $\sigma = -\nu$, give linearly-independent solutions. This is obvious, since the two solutions take the form[10]

$$y_1 = x^\nu \sum_{n\ge 0} a_n\, x^n\,, \qquad y_2 = x^{-\nu} \sum_{n\ge 0} \tilde a_n\, x^n\,. \tag{4.107}$$

Clearly, the prefactors $x^{\pm\nu}$ around the front of the (analytic) Taylor expansions are different fractional powers of x, and so obviously there is no linear relation between the solutions. For example, if $\nu = \frac{1}{3}$ then y_1 has terms $x^{1/3}$, $s^{4/3}$, etc, whilst y_2 has terms $x^{-1/3}$, $x^{2/3}$, etc.

This argument demonstrating the linear independence of the two solutions could clearly fail if ν were an integer or half-integer. Let us look at a specific example, where $\nu = 1$. We see from (4.102) that we shall have

$$\tilde a_{n+2} = -\frac{\tilde a_n}{n(n+2)} \tag{4.108}$$

for the putative "second solution" in (4.107). The first thing to notice is that we cannot use this equation to give us $\tilde a_2$ in terms of $\tilde a_0$, since there is a zero in the denominator on the right-hand side when $n = 0$. Thus we must conclude that $\tilde a_0 = 0$. Since we also have $\tilde a_1 = 0$ from (4.105), it means that the series for y_2 in (4.107) begins with the $\tilde a_2$ term.

[10]We use $\tilde a_n$ to distinguish the series expansion coefficients for the second solution from those for the first solution. Like the coefficients a_n in the first solution, they satisfy the recursion relation (4.102) too, but since $\sigma = -\nu$ rather than $\sigma = +\nu$, the actual expressions fr=or the $\tilde a_n$ will differ from those for the a_n.

The subsequent $\tilde{a}_n$ with n even are non-vanishing, while the $\tilde{a}_n$ with n odd vanish (since $\tilde{a}_1$ vanishes).

Now, we can perform the following relabelling; let $\tilde{a}_n = c_{n-2}$. Then we shall have

$$y_2 = \sum_{n\ge 2} \tilde{a}_n\, x^{n-1} = \sum_{n\ge 0} c_n\, x^{n+1}\,, \tag{4.109}$$

where in the second expression we have made the replacement $n \to n+2$ in the summation variable. From (4.108), it follows that $c_n = -c_{n-2}/(n(n+2))$, or in other words

$$c_{n+2} = -\frac{c_n}{(n+2)(n+4)}\,. \tag{4.110}$$

Of course since we had $\tilde{a}_2 \ne 0$ and $\tilde{a}_3 = 0$, we have $c_0 \ne 0$ and $c_1 = 0$.

Now, finally, let us compare with our first solution, y_1 in (4.107). Recalling that we are taking the example $\nu = 1$, we see from (4.102) that we have

$$y_1 = \sum_{n\ge 0} a_n\, x^{n+1}\,, \qquad a_{n+2} = \frac{a_n}{(n+2)(n+4)}\,, \tag{4.111}$$

with $a_0 \ne 0$ and $a_1 = 0$. Thus our supposed "second solution" y_2, given by (4.109) and (4.110), is exactly the same series, with coefficients c_n satisfying the identical recursion relation, as the first solution (4.111). This proves, for the example $\nu = 1$, that we fail to get the second solution in the form (4.99). A similar discussion shows that this happens whenever ν is an integer or half-integer. (That is, it happens whenever the difference of the two roots of the indicial equation, namely

$$\nu - (-\nu)\,, \tag{4.112}$$

is an integer.

From the earlier general discussion, we know that if the difference of the two roots of the indicial equation is an integer, we should expect that the linearly-independent second solution will involve a log term, as in (4.93). In our example of the Bessel equation, we should therefore look for a second solution of the form

$$y(x) = y_1(x)\, \log x + \sum_{n\ge 0} b_n\, x^{n-\nu}\,, \tag{4.113}$$

where $y_1(x)$ is the previously-obtained first solution, given in (4.107). We now plug (4.113) into the Bessel equation (4.98), and solve for the new coefficients b_n. (We can take it, for the purposes of this discussion, that we have already solved for the expansion coeffcients a_n in the first solution $y_1(x)$.)

The first thing to notice is that all the terms involving $\log x$ will automatically cancel out. This is because they will give

$$\Big(x^2\, y_1'' + x\, y_1' + (x^2 - \nu^2)\, y_1\Big)\, \log x\,, \tag{4.114}$$

which is zero precisely because y_1 is already known to satisfy the Bessel equation. The remaining terms, after multiplying by x^ν for convenience, give

$$2 \sum_{n\ge 0} (n+\nu)\, a_n\, x^{n+2\nu} + \sum_{n\ge 0} n\,(n-2\nu)\, b_n\, x^n + \sum_{n\ge 0} x^{n+2} = 0\,. \tag{4.115}$$

As usual, the task is to collect the coefficients of each power of x, and equate each such coefficient to zero. Notice that this only makes sense if 2ν is an integer. If we had 2ν not equal to an integer, then all the terms in the first summation would have to vanish independently of the terms in the remaining summations. This would imply that the a_n all vanished, which would contradict the fact that the coeffcients a_n in the first solution y_1 in (4.107) do not vanish. All that this means, of course, is that the second solution *does not* involve a $\log x$ if 2ν is not an integer; we already got a perfectly good second solution as in (4.107) when 2ν was not an integer, so we definitely should not expect a "third" solution with a $\log x$ term in this case! On the other hand, when 2ν *is* an integer, we can see from (4.115) that the terms in the first summation will combine with those in the second and third summations, giving us sensible equations that determine the coefficients b_n.

To illustrate what is going on, let us again consider our example of $\nu = 1$. Equation (4.115) becomes

$$2 \sum_{n\ge 0} (n+1)\, a_n\, x^{n+2} + \sum_{n\ge 0} n\,(n-2)\, b_n\, x^n + \sum_{n\ge 0} x^{n+2} = 0\,. \tag{4.116}$$

Relabelling $n \longrightarrow n+2$ in the second term, we then get

$$\sum_{n\ge 0} [2(n+1)\, a_n + b_n + n\,(n+2)\, b_{n+2}]\, x^{n+2} - b_1\, x = 0\,. \tag{4.117}$$

(As usual, after the relabelling we have to add in "by hand" the terms that have dropped off the bottom in the new summation over $n \ge 0$. In this case there is only one such term (the former $n = 1$ term), since at $n = 0$ the $n\,(n+2)$ prefactor gives zero.)

From (4.117), we obtain the recursion relation

$$b_{n+2} = -\frac{b_n + 2(n+1)\, a_n}{n\,(n+2)}\,, \qquad n \ge 0\,, \tag{4.118}$$

and also

$$b_1 = 0\,. \tag{4.119}$$

Looking at (4.118), we see that it will only make sense when $n = 0$ if we have

$$b_0 = -2a_0\,, \tag{4.120}$$

since otherwise we will get infinity from the n factor in the denominator. This means that b_2 is not determined by (4.118). (Look back to (4.117), before we divided out to get (4.118), to see that with $b_0 = -2a_0$ we get a consistent equation at order x^2, but that it tells us nothing about the value of b_2.)

The undetermined value for b_2 should not be a surprise. Our trial series solution (4.113) for the second solution is going to give us the most general possible expression for the linearly-independent second solution. In particular, it will produce for us a second solution that can include an arbitrary constant multiple of the first solution. That arbitrariness of adding in any constant multiple of the first solution must manifest itself in an arbitrariness in the solution for the b_n coefficients. And that is what we have just encountered. Why did it show up in an arbitrariness in the value of b_2? The reason is because we are looking at the example where $\nu = 1$. The first solution, y_1 in (4.107), has terms in $(a_0\,x, a_1\,x^2, a_2\,x^3, \ldots)$. The terms in our trial second solution (4.113), coming from the sum over $b_n\,x^{n-\nu}$ will have terms in $(b_0\,x^{-1}, b_1\,b_2\,x, b_3\,x^2, \ldots)$. Thus we see that the admixture of the first solution that we expect to see appearing when we construct the second solution in (4.113) will precisely begin with the term b_2.

The bottom line from the above discussion is that we can take b_2 to be anything we like; different values correspond to different admixtures of the first solution y_1 added in to our new second solution. It doesn't matter how much of y_1 one adds in; our second solution will still be linearly independent of y_1. The simplest choice, therefore, is to take $b_2 = 0$. We now have a complete specification of the second solution. It is given by (4.113), where we solve (4.118) for the coefficients b_n with $n \ge 3$, subject to

$$b_0 = -2a_0\,, \qquad b_1 = 0\,, \qquad b_2 = 0\,. \tag{4.121}$$

Clearly, a similar discussion could be given for any other choice of integer N such that $2\nu = N$. (This would include the case where $\nu = \frac{1}{2}$, whose discussion we deferred earlier.) We shall not dwell further on this here; it is to be hoped that the general idea of how one looks for series solutions of differential equations is now clear.

4.5 Sturm-Liouville Theory

4.5.1 Self-adjoint operators

In the previous sections, we discussed certain aspects of how to construct the solutions of second-order linear ODE's in considerable detail. Here, we shall take a look at some general properties of the solutions of the ODE. To begin, let us consider a general class of second-order differential operator $\mathcal{L}$, of the form

$$\mathcal{L}(u) = p_0(x)\, u'' + p_1(x)\, u' + p_2(x)\, u\,. \tag{4.122}$$

This is very much of the kind we discussed previously, as in (4.1), except that now we have a function of x multiplying the u'' term too. We shall assume that we are interested in studying this operator in some interval $a \le x \le b$, and that the functions $p_0(x)$, $p_1(x)$ and $p_2(x)$ are all real in this region. Furthermore, we assume that $p_0(x)$ does not vanish within the interval, i.e. for $a < x < b$, and $p_1(x)$ and $p_2(x)$ remain finite in the interval.[11] In other words, the equation $\mathcal{L}(u) = 0$ has no singular points within the interval, $a < x < b$. The points $x = a$ and $x = b$ themselves may be singular points, and indeed they commonly are.

Now, we may define the *adjoint* $\overline{\mathcal{L}}$ of the operator $\mathcal{L}$, as follows:

$$\begin{aligned} \overline{\mathcal{L}}(u) &\equiv \frac{d^2}{dx^2}(p_0\, u) - \frac{d}{dx}(p_1\, u) + p_2\, u \\ &= p_0\, u'' + (2p_0' - p_1)\, u' + (p_0'' - p_1' + p_2)\, u\,. \end{aligned} \tag{4.123}$$

The reason for introducing this operator can be seen from the following. Suppose we consider the integral

$$\int_a^b dx\, v\, \mathcal{L}u = \int_a^b dx\, v\, (p_0\, u'' + p_1\, u' + p_2\, u)\,, \tag{4.124}$$

and now integrate by parts to get the derivatives off u. Suppose that, for whatever reason, the boundary terms in the integrations by parts vanish, so that we can simply use the rule

$$\int dx f(x)\, g'(x) \longrightarrow -\int dx f'(x)\, g(x)\,. \tag{4.125}$$

In other words, we assume that our class of functions is such that

$$[f(x)\, g(x)]_a^b = 0\,. \tag{4.126}$$

Then, after integrating by parts twice on the first term in (4.124), and once on the second term, we shall have

$$\int_a^b dx ((p_0\, v)'' - (p_1\, v)' + p_2\, v)\, u\,, \tag{4.127}$$

[11] To complete all the technical specification, we shall assume that the first 2 derivatives of p_0 are continuous, the first derivative of p_1 is continuous, and that p_2 is continuous, for $a \le x \le b$.

and so

$$\int_a^b dx\, v\, \mathcal{L}u = \int_a^b dx (\overline{\mathcal{L}}v)\, u\,, \tag{4.128}$$

where $\overline{\mathcal{L}}$ is defined in equation (4.123). So the adjoint operator $\overline{\mathcal{L}}$ is the one that arises when we throw the derivatives over from the original operand function u and onto the function v that multiplies it in (4.124). We shall discuss later why we dropped the boundary terms.

It is clear that if the functions $p_i(x)$ are related to each other in an appropriate way, then the adjoint operator $\overline{\mathcal{L}}$ will in fact be identical to the original operator $\mathcal{L}$. From the second line in (4.123), we see that this will be true if it happens to be the case that p_0 and p_1 are related by

$$p_0'(x) = p_1(x)\,. \tag{4.129}$$

Then, we shall have

$$\overline{\mathcal{L}}u = \mathcal{L}u = p_0\, u'' + p_0'\, u' + p_2\, u = (p_0\, u')' + p_2\, u\,. \tag{4.130}$$

Now that we are down to just two function p_0 and p_2, we may as well give them names without indices, say $P(x)$ and $Q(x)$. Not surprisingly, an operator $\mathcal{L}$ that is equal to its adjoint $\overline{\mathcal{L}}$ is called a *self-adjoint operator*.

Note that *any* differential operator of the form (4.122), even if it is not itself self-adjoint, is related to a self-adjoint operator that is obtained by multiplying it by some appropriate function $h(x)$. To see, this, we note that the analogue of (4.129) for the operator multiplied by h will be $(h\, p_0)' = h\, p_1$, or in other words,

$$\frac{h'}{h} = \frac{p_1 - p_0'}{p_0}\,. \tag{4.131}$$

This equation can then simply be integrated to determine the required multiplying function h that will make the operator become self-adjoint. (Recall that we imposed the condition $p_0 \neq 0$ at the outset, so there is no problem in principle with performing the integration.) Thus we can proceed with our discussion by assuming that by this means, we have rendered our operator self-adjoint.

4.5.2 The Sturm-Liouville eigenvalue problem

Assuming now that we have a self-adjoint operator $\mathcal{L}$, we may consider the following eigenvalue problem,

$$\mathcal{L}u(x) + \lambda\, w(x)\, u(x) = 0\,, \tag{4.132}$$

where $w(x)$ is some given function, called a weight function or density function, and λ is a constant. It is assumed that $w(x) > 0$ in the interval $a \le x \le b$, except possibly for isolated points where $w(x) = 0$.

The idea is that we look for solutions $u(x)$, subject to certain boundary conditions imposed at $x = a$ and $x = b$. By analogy with the eigenvalue problem for a matrix M with eigenvectors V and eigenvalues λ

$$M\,V = \lambda\,V\,, \tag{4.133}$$

the solutions $u(x)$ to (4.132) are called eigenfunctions, and the corresponding constant λ is called the eigenvalue. The typical situation is that λ is an as-yet undetermined constant, and that one wants to find all the possible values λ for which the equation (4.132) admits solutions $u(x)$ that satisfy the specified boundary conditions. Commonly, it turns out that only a discrete (usually infinite) set of values of λ can occur.

We have met an example of such a Sturm-Liouville eigenvalue problem already in this course. Recall that we obtained the associated Legendre equation (2.28), by separating the Helmholtz equation in spherical polar coordinates. This equation is

$$((1-x^2)\,u')' - \frac{m^2}{1-x^2}\,u + \lambda\,u = 0\,, \tag{4.134}$$

which is clearly of the form (4.132), with

$$\mathcal{L}u = ((1-x^2)\,u')' - \frac{m^2}{1-x^2}\,u\,, \qquad w(x) = 1\,. \tag{4.135}$$

It is clear by comparing the form of $\mathcal{L}$ here with the general form in (4.130) that it is self-adjoint. When we solved for the solutions of the equation (actually, we considered the special case $m = 0$ for simplicity), we imposed the requirement that the functions $u(x)$ should be regular at $x = \pm 1$. We were in fact solving the Sturm-Liouville problem for the Legendre equation, seeking all the solutions in the interval $-1 \le x \le 1$ that are regular at the endpoints. We found that such eigenfunctions exist only if the eigenvalue λ takes the form $\lambda = \ell(\ell+1)$, where ℓ is a non-negative integer. The corresponding eigenfunctions $P_\ell(x)$ are the Legendre polynomials.

The example of the Legendre equation illustrates the typical way in which a Sturm-Liouville problem arises in physics. One separates an equation such as the Laplace equation, Helmholtz equation or wave equation, and obtains ODE's for functions in the various independent variables. The required solutions to these ODE's must satisfy certain boundary conditions, and one then looks for the allowed values of the separation constants for which regular solutions arise. Thus the eigenvalue in a Sturm-Liouville problem is typically a separation constant.

To proceed, let us return to the question of boundary conditions. Recall that we motivated the introduction of the adjoint operator $\overline{\mathcal{L}}$ in (4.123) by considering the integral $\int v\,\mathcal{L}u$, and throwing the derivatives over from u and onto v, by integration by parts. In the process, we ignored the possible contributions from the boundary terms arising from the integrations by parts, promising to return to discuss it later. This is what we shall now do. First of all, we should actually be a little more general than in the previous discussion, and allow for the possibility that the functions on which $\mathcal{L}$ acts might be complex. For any pair of functions u and v, we then define the *inner product* (v,u), as

$$(v,u) \equiv \int_a^b dx\, \bar v(x)\, u(x)\,, \tag{4.136}$$

where the bar on v denotes the complex conjugate.

Let's see what happens if we go through the details of integrating by parts, for the self-adjoint operator $\mathcal{L}$, defined by

$$\mathcal{L}u = (P(x)\, u')' + Q(x)\, u\,. \tag{4.137}$$

What we get is

$$\begin{aligned}
(v,\mathcal{L}u) &= \int_a^b dx\Big(\bar v\,(P\,u')' + \bar v\, Q\, u\Big)\\
&= \int_a^b dx\Big(-\bar v'\,(P\,u') + \bar v\, Q\, u\Big) + \Big[P\,\bar v\, u'\Big]_a^b\\
&= \int_a^b dx\Big((P\,\bar v')'\, u + \bar v\, Q\, u\Big) + \Big[P\,\bar v\, u' - P\,\bar v'\, u\Big]_a^b\,.
\end{aligned} \tag{4.138}$$

The integrand in the last line is just like the one in the first line, but with the roles of u and $\bar v$ interchanged. Thus if the boundary terms in the last line were to vanish, we would have established that

$$(v,\mathcal{L}u) = (\mathcal{L}v, u)\,. \tag{4.139}$$

We make the boundary terms vanish by fiat; i.e. we declare that the space of functions we shall consider will be such that the boundary terms vanish. One way to do this is to require that

$$P(a)\,\bar u_1(a)\, u_2'(a) = 0\,, \qquad P(b)\,\bar u_1(b)\, u_2'(b) = 0\,, \tag{4.140}$$

for *any* pair of eigenfunctions (possibly the same one) u_1 and u_2. In practice, we might achieve this by requiring, for example, that each eigenfunction satisfy

$$u(a) = u(b) = 0\,. \tag{4.141}$$

Another possibility is to require instead

$$u'(a) = u'(b) = 0 \tag{4.142}$$

for each eigenfunction. Yet a third possibility is to impose a weaker condition than (4.141), and require that each eigenfunction satisfy

$$P(a)\,u(a) = 0\,, \qquad P(b)\,u(b) = 0\,. \tag{4.143}$$

Any of these last three conditions will ensure that (4.140) is satisfied, and hence that the boundary terms from the integrations by parts give no contribution. Our Legendre equation analysis was an example where we were effectively imposing boundary conditions of the type (4.143). In that case we had $P(x) = (1 - x^2)$, and we required our eigenfunctions to be regular at $x = -1$ and $x = 1$. Therefore the $P(x)$ factor ensured that (4.140) was satisfied in that example.

A slightly more general way to make the boundary terms in the last line of (4.138) vanish is simply to require

$$P(a)\,\bar{u}_1(a)\,u_2'(a) = P(b)\,\bar{u}_1(b)\,u_2'(b)\,, \tag{4.144}$$

for all possible pairs of eigenfunctions u_1 and u_2, without demanding that this quantity itself be zero. Such a condition might naturally arise if the independent variable x represented a periodic coordinate, or else was effectively describing a periodic direction, such as a coordinate on an infinite lattice. Having imposed boundary conditions such that the boundary terms in the last line of (4.138) vanish, one says that the self-adjoint operator $\mathcal{L}$ is *Hermitean* with respect to the functions u and v that satisfy such boundary conditions. One should therefore keep in mind this distinction between the meaning of self-adjoint and Hermitean. Any operator $\mathcal{L}$ of the form (4.137) is self-adjoint. If in addition, one restricts attention to functions that satisfy the boundary conditions (4.140) or (4.144), then the operator $\mathcal{L}$ is Hermitean with respect to this class of eigenfunctions.

Note that we can actually extend the notion of Hermitean operators to include cases where operator itself is not built purely from real quantities. This situation arises, for example, in quantum mechanics. Consider, for instance, the momentum operator

$$p_x \equiv -\mathrm{i}\,\frac{d}{dx} \tag{4.145}$$

(we choose units where $\hbar = 1$ here, since Planck's constant plays an inessential rôle here). Let us assume that we impose boundary conditions on u and v (which would be called wave-functions, in this quantum-mechanical context) such that we can drop the boundary terms after integration by parts. Then we see that

$$(v, p_x\, u) = -\mathrm{i} \int_a^b dx\, \bar v\, u' = \mathrm{i} \int_a^b dx\, \bar v'\, u = (p_x\, v, u)\,. \tag{4.146}$$

Note that the sign worked out nicely in the end because $(p_x\, v, u)$ means, by virtue of the definition (4.136),

$$\int_a^b dx\, \overline{(p_x\, v)}\, u\,, \tag{4.147}$$

and so the complex conjugation of the $-\mathrm{i}$ factor in (4.145) produces $+\mathrm{i}$. Of course this example is a first-order operator, rather than being of the general class of second-order operators that we were previously discussing. The key point, though, is that we can extend the notion of hermiticity to any differential operator A, through the requirement $(v, A\, u) = (A\, v, u)$, where appropriate boundary conditions are imposed so that the boundary terms from the integrations by parts can be dropped.

4.5.3 Eigenfunctions of Hermitean Operators

We already alluded to the fact that there is a close analogy between the Sturm-Liouville eigenvalue problem for differential operators, and the eigenvalue problem in the theory of matrices. Before proceeding with the Sturm-Liouville problem, let us first briefly recall some of the features of the matrix eigenvalue problem.

Suppose that A is an Hermitean matrix, which we write as $A = A^\dagger$. By definition, $A^\dagger$ is the matrix obtained by transposing A, and complex conjugating its components. Suppose we are looking for eigenvectors V of the matrix A, namely vectors that satisfy the equation

$$A\, V = \lambda\, V\,, \tag{4.148}$$

where λ is some constant, called the eigenvalue. Let us suppose that A is an $N \times N$ matrix (it must, of course, be square, since we are requiring that it equal the complex conjugate of its transpose).

Rewriting (4.148) as

$$(A - \lambda \mathbb{1})\, V = 0\,, \tag{4.149}$$

where $\mathbb{1}$ means the unit $N \times N$ matrix, we know from the theory of linear algebra that the condition for solutions of this equation to exist is that

$$\det(A - \lambda \mathbb{1}) = 0\,. \tag{4.150}$$

This gives an N'th order polynomial equation for λ, called the *characteristic equation*, and thus we will have N roots, which we may call $\lambda_{(n)}$, for $1 \le n \le N$, and associated with each root will be the corresponding eigenvector $V_{(n)}$. In general, for an *arbitrary* square matrix A they could be complex. However here, since we are requiring that A be Hermitean, we can show that the eigenvalues $\lambda_{(n)}$ are real. We do this by taking the eigenvector equation (4.148) for a particular eigenvector $V_{(n)}$ and associated eigenvalue $\lambda_{(n)}$, and multiplying from the left by the Hermitean conjugate of $V_{(n)}$:

$$V_{(n)}^\dagger\, A\, V_{(n)} = \lambda_{(n)}\, V_{(n)}^\dagger\, V_{(n)}\,. \tag{4.151}$$

Now, take the Hermitean conjugate of this expression, recalling that for matrices X and Y we have $(XY)^\dagger = Y^\dagger\, X^\dagger$. Thus we get

$$V_{(n)}^\dagger\, A^\dagger\, V_{(n)} = \bar\lambda_{(n)}\, V_{(n)}^\dagger\, V_{(n)}\,. \tag{4.152}$$

Since we are assuming A is Hermitean, this gives

$$V_{(n)}^\dagger\, A\, V_{(n)} = \bar\lambda_{(n)}\, V_{(n)}^\dagger\, V_{(n)}\,. \tag{4.153}$$

Subtracting this from (4.151), we get

$$(\lambda_{(n)} - \bar\lambda_{(n)})\, V_{(n)}^\dagger\, V_{(n)} = 0\,. \tag{4.154}$$

Bearing in mind that $V_{(n)}^\dagger\, V_{(n)}$ equals the sum of the modulus-squares of all the components of $V_{(n)}$, i.e. $V^\dagger\, V = \sum_i \bar V_i\, V_i$, we see that for any non-zero vector $V_{(n)}$ (which we have), (4.154) implies that

$$\bar\lambda_{(n)} = \lambda_{(n)}\,, \tag{4.155}$$

and hence all the eigenvalues of an Hermitean matrix are real.

By a small extension of the previous procedure, one can show also that if two eigenvectors $V_{(n)}$ and $V_{(m)}$ have unequal eigenvalues, $\lambda_{(n)} \ne \lambda_{(m)}$, then the eigenvectors are orthogonal to each other, meaning $V_{(n)}^\dagger\, V_{(m)} = 0$. To show this, we take the eigenvector equation (4.148) for $V_{(m)}$, i.e. $A\, V_{(m)} = \lambda_{(m)}\, V_{(m)}$, and multiply on the left by $V_{(n)}^\dagger$. From this we subtract the equation obtained by Hermitean conjugating $A\, V_{(n)} = \lambda_{(n)}\, V_{(n)}$ and multiplying on the right by $V_{(m)}$:

$$V_{(n)}^\dagger\, A\, V_{(m)} - V_{(n)}^\dagger\, A\, V_{(m)} = 0 = (\lambda_{(m)} - \lambda_{(n)})\, V_{(n)}^\dagger\, V_{(m)}\,, \tag{4.156}$$

where we have made use of $A^\dagger = A$, the already-established fact that $\bar\lambda_{(n)} = \lambda_{(n)}$. In the case where two different eigenvectors $V_{(1)}$ and $V_{(2)}$ happen to have the *same* eigenvalue λ (i.e. they are *degenerate*), then it means that we have a two-dimensional space of eigenvectors $U \equiv a\,V_{(1)} + b\,V_{(2)}$ which satisfy $A\,U = \lambda\,U$ for arbitrary constants a and b. Clearly, we can always choose two members from this family, say U_1 and U_2, by judicious choice of the constants a and b, such that $U_1^\dagger\,U_2 = 0$. This can easily be generalised to a scheme, known as *Gram-Schmidt Orthogonalisation*, for dealing with arbitrary numbers of degenerate eigenvalues.

Thus either by necessity, in the case of non-degenerate eigenvalues, supplemented by choice, in the case of degenerate eigenvalues, we can arrange always that the set of N eigenvectors are orthogonal,

$$V_{(n)}^\dagger\,V_{(m)} = 0\,, \qquad m \ne n\,. \tag{4.157}$$

Of course we can easily arrange also to make each eigenvector have unit length, $V_{(n)}^\dagger\,V_{(n)} = 1$, by rescaling it if necessary. Thus we can always choose the eigenvectors to be *orthonormal*:

$$V_{(n)}^\dagger\,V_{(m)} = \delta_{nm}\,, \tag{4.158}$$

for all m and n.

After this interlude on the eigenvalue problem for Hermitean matrices, let us return now to the Sturm-Liouville theory for Hermitean differential operators. As we already saw, the problem here is to study the eigenvalues λ and eigenfunctions u for the operator equation

$$\mathcal{L}u(x) + \lambda\,w(x)\,u(x) = 0\,, \tag{4.159}$$

where $\mathcal{L}$ is an Hermitean operator and $w(x)$ is called the weight function. It will be assumed that $w(x)$ is non-negative in the interval $a \le x \le b$, and in fact that $w(x) > 0$ except possibly for isolated points where $w(x) = 0$.

We can now rerun the previous derivations for Hermitean matrices in the case of our Hermitean Sturm-Liouville operator $\mathcal{L}$. To economise on the writing, recall that we are defining the *inner product* (v, u) of any functions u and v by

$$(v, u) \equiv \int_a^b dx\,\bar v(x)\,u(x)\,. \tag{4.160}$$

Note that it follows immediately from this definition that we shall have

$$\overline{(v, u)} = (u, v)\,, \tag{4.161}$$

and that if f is any *real* function,

$$(v, f\,u) = (f\,v, u)\,. \tag{4.162}$$

Of course it is also the case that any *constant* factor a can be pulled outside the integral, and so

$$(v, a\,u) = a\,(v,u)\,, \qquad (a\,v, u) = \bar{a}\,(v,u)\,. \tag{4.163}$$

Note that we are allowing for the possibility that a is complex; the complex conjugation of a in the second equation here is an immediate consequence of the definition (4.160) of the inner product.

Further properties of the inner product are that for any function u, we shall have

$$(u,u) \ge 0\,, \tag{4.164}$$

since we are integrating the quantity $|u(x)|^2$, which is pointwise non-negative, over the interval $a \le x \le b$. In fact, the only way that (u,u) can equal zero is if $u(x) = 0$ for all x in the interval $a \le x \le b$. More generally, if f is a positive function in the interval $[a,b]$, we shall have

$$(u, f\,u) \ge 0\,, \tag{4.165}$$

with equality achieved if and only if $u = 0$.

Recall also that the Sturm-Liouville operator $\mathcal{L}$, being Hermitean, satisfies

$$(v, \mathcal{L}\,u) = (\mathcal{L}\,v, u)\,. \tag{4.166}$$

Now, suppose that we have eigenfunctions u_n with eigenvalues λ_n for the Sturm-Liouville problem (4.159):

$$\mathcal{L}\,u_n + \lambda_n\,w\,u_n = 0\,. \tag{4.167}$$

Consequently, we have

$$(u_m, \mathcal{L}\,u_n) + \lambda_n\,(u_m, w\,u_n)\,. \tag{4.168}$$

Now we complex conjugate this equation, getting

$$\begin{aligned} 0 &= \overline{(u_m, \mathcal{L}\,u_n)} + \bar{\lambda}_n\,\overline{(u_m, w\,u_n)} = \\ &= (\mathcal{L}\,u_n, u_m) + \bar{\lambda}_n\,(w\,u_n, u_m) \\ &= (u_n, \mathcal{L}\,u_m) + \bar{\lambda}_n\,(u_n, w\,u_m)\,, \end{aligned} \tag{4.169}$$

where we have made use of various of the properties of the inner product detailed above, and the Hermiticity of $\mathcal{L}$. By interchanging the indices m and n, this last line tells us that

$$(u_m, \mathcal{L}\,u_n) + \bar{\lambda}_m\,(u_m, w\,u_n) = 0\,. \tag{4.170}$$

Subtracting this from (4.168), we therefore find that

$$(\lambda_n - \bar{\lambda}_m)\,(u_m, w\,u_n) = 0\,. \tag{4.171}$$

(This treatment is precisely analogous to the one we followed for the case of Hermitean matrices. We have just shortened the argument a bit here, by handling the $n = m$ and $n \neq m$ cases all in one go. We could have done the same for the matrix case.)

Consider first the case where we take $m = n$, giving

$$(\lambda_n - \bar{\lambda}_n)\,(u_n, w\,u_n) = 0\,. \tag{4.172}$$

Now, our foresight in insisting that the weight function $w(x)$ be non-negative in the interval $[a, b]$ becomes apparent, since it means that for a non-vanishing eigenfunction u_n we shall have $(u_n, w\,u_n) > 0$. Thus equation (4.172) implies that

$$\bar{\lambda}_n = \lambda_n\,, \tag{4.173}$$

and so all the eigenvalues in the Sturm-Liouville problem are real.

Using the reality of the λ_n, we can now rewrite (4.171) as

$$(\lambda_n - \lambda_m)\,(u_m, w\,u_n) = 0\,. \tag{4.174}$$

Thus if two eigenfunctions u_m and u_n have unequal eigenvalues, $\lambda_m \neq \lambda_n$, then we can deduce that they are *orthogonal*, by which we mean

$$(u_m, w\,u_n) = 0\,. \tag{4.175}$$

As in the analogous matrix case, if there is a degeneracy of eigenfunctions, for example with two eigenfunctions u_1 and u_2 having the same eigenvalue λ, then it follows that any linear combination $U = \alpha\,u_1 + \beta\,u_2$ will satisfy the equation (4.159), for arbitrary constants α and β. We can clearly always choose two pairs of constants α_1, β_1 and α_2, β_2, defining two combinations $U_1 = \alpha_1\,u_1 + \beta_1\,u_2$ and $U_2 = \alpha_2\,u_1 + \beta_2\,u_2$, such that we arrange that $(U_1, w\,U_2) = 0$. This process can be extended to deal with arbitrary numbers of degenerate eigenfunctions, in the operator version of the Gram-Schmidt orthogonalisation procedure.

In order not to become too abstract, let us pause at this point to consider a simple example. It will also serve to illustrate an important feature of a typical Sturm-Liouville problem, which we have been tacitly assuming so far without comment. Namely, we have been labelling our eigenfunctions by an subscript n, with the implication that n is some integer that enumerates the set of eigenfunctions. In other words, we seem to have been assuming that there is a discrete set of eigenfunctions, although we have not yet addressed the question of how many there are. In fact, for the kind of situation we are considering, with boundary conditions of the form (4.140) or (4.144), the set of eigenfunctions u_n will indeed be discrete, so that we can sensibly label them by an integer n. The number of eigenfunctions is infinite, so we can think of the label n as running from 1 to ∞.

Let's see how this works in an example. Take the operator $\mathcal{L}$ and the weight function $w(x)$ to be

$$\mathcal{L} = \frac{d^2}{dx^2}\,, \qquad w(x) = 1\,. \tag{4.176}$$

It is clear that this operator $\mathcal{L}$ is indeed self-adjoint. The Sturm-Liouville problem in this example is therefore to study the eigenvalues and eigenfunctions of the equation

$$u'' + \lambda\, u = 0\,. \tag{4.177}$$

Of course this equation is so easy that we can solve it in our sleep:

$$u(x) = A\, \cos \lambda^{\frac{1}{2}}\, x + B\, \sin \lambda^{\frac{1}{2}}\, x\,. \tag{4.178}$$

Now, we have to consider boundary conditions. Suppose for example, that we choose our interval to be $0 \le x \le \pi$, so $a = 0$, $b = \pi$. One choice for the boundary conditions would be to require

$$u(0) = 0\,, \qquad u(\pi) = 0\,, \tag{4.179}$$

in which case we would deduce that the eigenvalues λ must take the form

$$\lambda_n = n^2\,, \tag{4.180}$$

where n is an integer, and the allowed eigenfunctions would be

$$U_n = \sin nx\,. \tag{4.181}$$

We see here a discrete infinity of eigenfunctions and eigenvalues.

Of course these boundary conditions are a bit of an overkill, since we really need only demand that the boundary terms from the integrations by parts vanish, and their vanishing will be ensured if the periodic boundary conditions (4.144) are satisfied, which amounts to

$$\bar v(a)\, u'(a) = \bar v(b)\, u'(b) \tag{4.182}$$

for *any* pair of eigenfunctions u and v (including, possibly, the *same* eigenfunction for u and v), since the function $P(x) = 1$. Now, we can see that the set of functions $\sin 2nx$ and $\cos 2nx$ will all be satisfactory eigenfunctions. Let us give these names,

$$U_n = \sin 2nx\,, \qquad V_n = \cos 2nx\,. \tag{4.183}$$

Thus for any choice of any two functions u and v taken from this total set, it will always be the case that

$$v(0)\, u'(0) = v(\pi)\, u'(\pi)\,. \tag{4.184}$$

(A non-trivial case to check here is when $u = V_n$ and $v = U_m$.) Note that now the two eigenfunctions U_n and V_n have the *same* eigenvalue $\lambda_n = 4n^2$.

4.5.4 Eigenfunction expansions

The example we have just looked at, where $\mathcal{L} = \frac{d^2}{dx^2}$, and indeed the example of the Legendre equation that we considered earlier, illustrate some general features of the eigenfunctions and eigenvalues of any Sturm-Liouville operator of the kind we are considering. These features can be shown to be true in general, but since the proofs are slightly intricate and long-winded, we shall not present them here, but merely state them. The statements are as follows, for any Sturm-Liouville operator with $a \le x \le b$, where $b - a$ is finite, and appropriate boundary conditions imposed at $x = a$ and $x = b$ (we shall specify what is appropriate below):

1. There is always a *lowest* eigenvalue, which we shall call λ_1.

2. There is a non-zero gap between each eigenvalue and the next largest one. Thus we may order them

$$\lambda_1 < \lambda_2 < \lambda_3 < \cdots\,. \tag{4.185}$$

   The gap can never become infinitesimal, for any $\lambda_{n+1} - \lambda_n$, no matter how large n is. (Assuming, as we are, that $b - a$ is finite.)

3. Consequently, the eigenvalues increase without bound; there is no "largest" eigenvalue, and eigenvalues occur that are larger than any given finite value.

4. The number of nodes in the eigenfunction u_n increases with increasing n. In other words, the function u_n oscillates more and more rapidly with increasing n.

Let us deal straight away with the issue of what is meant by "appropriate boundary conditions." In particular, notice that Property 2 here is not satisfied by the $\mathcal{L} = \frac{d^2}{dx^2}$ example with the periodic boundary conditions (4.184), although it is satisfied in the case of the more stringent boundary condition (4.179) we considered previously. The point is that the slightly less restrictive boundary conditions of the periodic type tend to allow both independent solutions of the second-order ODE at a fixed value of λ, whereas the more forceful conditions like (4.179) tend to allow only one of the two solutions. So there is commonly a two-fold degeneracy of eigenvalues when the weaker kinds of boundary condition are imposed. It is perfectly straightforward to accommodate this in some appropriate generalisations of the properties listed above, but it is once again one of those examples where one can spend time endlessly dotting all the i's and crossing all the t's, and at the end of the day one has not really added hugely to the understanding of the key points. Let us assume for now that we choose sufficiently powerful boundary conditions that the degeneracies are avoided.

Now, to proceed, let us consider the following problem. It is familiar from the theory of Fourier series that if we have an arbitrary function $f(x)$ defined in the interval $0 \le x \le \pi$, such that $f(0) = 0$ and $f(\pi) = 0$, we can expand it in terms of the functions $\sin nx$, as

$$f(x) = \sum_{n\ge 1} c_n \sin nx\,, \tag{4.186}$$

where

$$c_n = \frac{2}{\pi}\int_0^\pi dx\, f(x)\, \sin nx\,. \tag{4.187}$$

Since we have seen that the functions $\sin nx$ arise as the eigenfunctions of the Sturm-Liouville problem with $\mathcal{L} = \frac{d^2}{dx^2}$, with the boundary conditions $u(0) = u(\pi) = 0$, it is natural to suppose that we should be able to carry out analogous series expansions in terms of the eigenfunctions for other Sturm-Liouville operators. This is the subject we shall now pursue.

Let us begin by supposing that we can indeed expand an arbitrary function $f(x)$, satisfying our chosen Sturm-Liouville boundary conditions, in terms of the eigenfunctions u_n:

$$f(x) = \sum_{n\ge 1} c_n\, u_n(x)\,. \tag{4.188}$$

Using the orthonormality of the eigenfunctions u_n, i.e. $(u_m, w\, u_n) = \delta_{mn}$, it follows that

$$\begin{aligned} (u_m, w\, f) &= \sum_{n\ge 0} c_n\, (u_m, w\, u_n)\,, \\ &= \sum_{n\ge 1} c_n\, \delta_{mn}\,, \\ &= c_m\,. \end{aligned} \tag{4.189}$$

Thus we have solved for the coefficients c_n in the expansion (4.188),

$$c_n = (u_n, w\, f) \equiv \int_a^b dx\, w(x)\, f(x)\, \bar u_n(x)\,. \tag{4.190}$$

Is this the end of the story? Well, not quite. We have tacitly assumed in the above discussion that it is *possible* to make an expansion of the form (4.188). The question of whether or not it is actually possible is the question of whether or not the eigenfunctions u_n form a *complete set.* Think of the analogous question for finite-dimensional vectors. What constitutes a complete set of basis vectors in an N-dimensional vector space? The answer is you need N independent basis vectors, which can span the entire space. In terms of these, you can expand *any* vector in the space. For example, in three-dimensional Cartesian space we can use the three unit vectors lying along the x, y and z axes as basis vectors; they form a complete set.

The problem in our present case is that we effectively have an infinite-dimensional vector space; there are infinitely many independent eigenfunctions. Certainly, we know that a complete set of basis functions must be infinite in number. We indeed have infinitely many functions u_n, the eigenfunctions of the Sturm-Liouville problem. But is it a "big enough" infinity? This is the question we need to look at in a little bit of detail. It is worth doing because it lies at the heart of so many techniques that one uses in physics. Think of quantum mechanics, for example, where one expands an arbitrary wave function in terms of the eigenfunctions of the Schrödinger equation. To do this, one needs to be sure one has a complete set of basis functions. It is the same basic question as the one we shall look at here for the Sturm-Liouville problem. To do so, we first need to study a another aspect of Sturm-Liouville theory:

A Variational Principle for the Sturm-Liouville Equation:

To begin, we note that the Sturm-Liouville equation $\mathcal{L}u + \lambda\, w\, u = 0$, with $\mathcal{L}u \equiv (P(x)\, u')' + Q(x)\, u$, can be derived rather elegantly from a variational principle. Define the functional[12] $\Omega(f)$ for any function $f(x)$, by

$$\Omega(f) \equiv (f', P\, f') - (f, Q\, f) = \int_a^b dx\, (P\, f'^2 - Q\, f^2)\,. \tag{4.191}$$

(We shall, for simplicity, assume for now that we deal with *real* functions. There is no great subtlety involved in treating complex functions; essentially we would just write $|f|^2$ in place of f^2, *etc.*. It is just a bit simpler to let them be real, and no great point of principle will be lost. Redo all the steps for complex functions if you wish.) Let us also define the

[12] "Functional" is just a fancy name for an operator that takes a function as its argument, and produces a number from it.

norm-squared of the function f:

$$\mathcal{N}(f) \equiv (f, w\, f) = \int_a^b dx\, w(x)\, (f(x))^2\,, \tag{4.192}$$

It is useful also to define more general *bilinear* functionals $\Omega(f,g)$ and $\mathcal{N}(f,g)$, by

$$\begin{aligned} \Omega(f,g) &\equiv (f', P\, g') - (f, Q\, g)\,, \\ \mathcal{N}(f,g) &= \equiv (f, w\, g)\,. \end{aligned} \tag{4.193}$$

Comparing with (4.191) and (4.192), we see that $\Omega(f) = \Omega(f,f)$, and $\mathcal{N}(f) = \mathcal{N}(f,f)$. Note that other properties of these functionals are

$$\begin{aligned} \mathcal{N}(f,g) &= \mathcal{N}(g,f)\,, \\ \mathcal{N}(f+g) &= \mathcal{N}(f) + \mathcal{N}(g) + 2\mathcal{N}(f,g)\,, \\ \Omega(f,g) &= \Omega(g,f)\,, \\ \Omega(f+g) &= \Omega(f) + \Omega(g) + 2\Omega(f,g)\,, \\ \Omega(f,g) &= -(f, \mathcal{L}g) = -(\mathcal{L}f, g)\,, \end{aligned} \tag{4.194}$$

where as usual $\mathcal{L}$ is the Sturm-Liouville operator, $\mathcal{L}u = (P\, u')' + Q\, u$. Note that in deriving the last line, we must assume that the functions f and g satisfy our Sturm-Liouville boundary conditions, so the boundary terms from integrations by parts can be dropped. All functions that we shall consider from now on will be assumed to satisfy these boundary conditions. We shall sometimes refer to them as *admissible functions.*

We shall now show how the eigenfunctions and eigenvalues of the Sturm-Liouville problem can be built up, one by one, by considering the following minimisation problem. We start by looking for the function f, subject to some specified Sturm-Liuoville boundary conditions, that minimises the ratio

$$R(f) \equiv \frac{\Omega(f)}{\mathcal{N}(f)} = \frac{\int_a^b dx\, [P\, f'^2 - Q\, f^2]}{\int_a^b dx\, w\, f^2}\,, \tag{4.195}$$

(Of course f can be determined only up to a constant scaling, since the ratio in is invariant under $f(x) \longrightarrow k\, f(x)$, where k is any constant. Thus it will always be understood that when we speak of "the minimising function," we mean modulo this scaling arbitrariness.)

To get an overview of the idea, consider first the following simple argument. Let us suppose that we make small variations of f, i.e. we replace f by $f + \delta f$, where the variations will be assumed also to be subject to the same Sturm-Liouville boundary conditions. (In other words, we consider small variations that keep us within the same class of boundary conditions.) We shall work only to first order in the small variation δf. With $R(f)$ defined in (4.195), we therefore have

$$\delta R = \frac{\delta\Omega}{\mathcal{N}} - \frac{\Omega}{\mathcal{N}^2}\,\delta\mathcal{N}\,, \tag{4.196}$$

where for any functional $X(f)$ we define its variation by

$$\delta X(f) \equiv X(f+\delta f) - X(f)\,. \tag{4.197}$$

Now we shall have

$$\begin{aligned}
\delta\Omega(f) &= \int_a^b dx\,(-2P\,f'\,\delta f' + 2Q\,f\,\delta f)\,,\\
&= \int_a^b dx\,[2(P\,f')\,\delta f + 2Q\,f\,\delta f] - 2\Big[P\,f'\,\delta f\Big]_a^b\,,\\
&= 2\int_a^b dx\,[(P\,f')\,\delta f + Q\,f\,\delta f]\,.
\end{aligned}\tag{4.198}$$

Note that the boundary terms drop out because, by supposition, f and δf both satisfy the given Sturm-Liouville boundary conditions. Likewise, we have, without any need for integration by parts,

$$\delta\mathcal{N}(f) = 2\int_a^b dx\,w\,f\,\delta f\,. \tag{4.199}$$

Now substitute into (4.196), and choose $f = f_0$, the function that supposedly minimises $R(f)$. Defining $R_0 \equiv R(f_0)$, we shall therefore have

$$\delta R = -\frac{2}{\mathcal{N}(f_0)}\int_a^b dx\,[(P\,f_0')' + Q\,f_0 + R_0\,w\,f_0]\,\delta f\,. \tag{4.200}$$

But if $R(f)$ is minimised by taking $f = f_0$, it must be that to first order in varition around $f = f_0$, i.e. for $f = f_0 + \delta f$, we must have $\delta R = 0$. This is obvious from the following argument: Suppose a given variation δf made δR non-zero at first order. Since $R(f)$, and hence δR, is just a number, then we would either have δR is positive or δR is negative. If it were negative, then this would be an immediate contradiction to the statement that $f = f_0$ is the function that minimises $R(f)$, and so this is impossible. Suppose δR were instead positive. But now, we could just take a new δf that is the negative of the original δf; now we would find that for a variation $-\delta f$, we again had δR negative, and again we would have a contradition. Therefore, the only possible conclusion is that if $R(f_0)$ is the minimum value of $R(f)$, then $\delta R = 0$ to first order in δf.

Recall that we placed no conditions on δf, other than that it should satisfy specified Sturm-Liouville boundary conditions at $x = a$ and $x = b$. Since it is otherwise arbitrary in the interval $a < x < b$, it follows that (4.200) can only be zero for all possible suche δf if the integrand itself vanishes, i.e.

$$(P\, f_0')' + Q\, f_0 + R_0\, w\, f_0 = 0\,. \tag{4.201}$$

This shows that the function f_0 that minimises $R(f)$ subject to the given Sturm-Liouville boundary conditions is itself an eigenfunction of the Sturm-Liouville problem, with eigenvalue $R_0 = R(f_0)$. Thus we see that by minimising $R(f)$ defined in (4.195), we obtain the eigenfunction with the lowest eigenvalue, and we determine this eigenvalue.

Notice that this can provide a useful way of getting an estimate on the lowest eigenvalue of the Sturm-Liouville problem. Even if the Sturm-Liouville operator is complicated and we cannot explicitly solve for the eigenfunctions in the equation

$$(P\, u')' + Q\, u + \lambda\, w\, u = 0\,, \tag{4.202}$$

we can just make a *guess* at the lowest eigenfunction, say $u = \tilde{u}$. Of course we should make sure that our guessed function $\tilde{u}$ does at least satisfy the given Sturm-Liouville boundary conditions; that is easily done. We then evaluate $R(\tilde{u})$, defined in (4.195). By our argument above, we therefore know that

$$R(\tilde{u}) \ge \lambda_1\,, \tag{4.203}$$

where λ_1 is the lowest eigenvalue of the Sturm-Liouville problem. If we were lucky enough to guess the exact lowest eigenfunction, then we would have $R(\tilde{u}) = \lambda_1$. In the more likely event that our guessed function $\tilde{u}$ is not the exact eigenfunction, we shall have $\mathbb{R}(\tilde{u}) > \lambda_1$. The nearer $\tilde{u}$ is to being the true lowest eigenfunction, the nearer $R(\tilde{u})$ will be to the true lowest eigenvalue. We can keep trying different choices for $\tilde{u}$, until we have made $R(\tilde{u})$ as small as possible. This will give us an upper bound on the lowest eigenvalue.

Let us now look at the variational problem in a bit more detail. As we shall see, we can actually do quite a bit more, and learn also about the higher eignfunctions and eigenvalues also.

Suppose now that we call the function that minimises $R(f)$ ψ_1, and that the minimum value for R in 4.195 is R_1, so

$$\Omega(\psi_1) = R_1\, \mathcal{N}(\psi_1)\,. \tag{4.204}$$

Then by definition it must be that

$$\Omega(\psi_1 + \epsilon\, \eta) \ge R_1\, \mathcal{N}(\psi_1 + \epsilon\, \eta)\,. \tag{4.205}$$

Here, ϵ is an arbitrary constant, and η is any function that satisfies the Sturm-Liouville boundary conditions. Thus from the various properties of $\mathcal{N}$ and Ω given above, we see that

$$\Omega(\psi_1) + 2\epsilon\,\Omega(\psi_1,\eta) + \epsilon^2\,\Omega(\eta) \ge R_1\,\mathcal{N}(\psi) + 2\epsilon\,R_1\,\mathcal{N}(\psi_1,\eta) + \epsilon^2\,R_1\,\mathcal{N}(\eta)\,. \tag{4.206}$$

Now, by definition we have $\Omega(\psi_1) = R_1\,\mathcal{N}(\psi_1)$, and so the terms independent of ϵ in this inequality cancel. We are left with

$$2\epsilon\,[\Omega(\psi_1,\eta) - R_1\,\mathcal{N}(\psi_1,\eta)] + \epsilon^2\,[\Omega(\eta) - R_1\,\mathcal{N}(\eta)] \ge 0\,. \tag{4.207}$$

Now, by taking ϵ sufficiently small (so that the ϵ^2 terms become unimportant) and of the proper sign, we could clearly violate this inequality unless the coefficient of the ϵ term vanishes. Thus we deduce that

$$\Omega(\psi_1,\eta) - R_1\,\mathcal{N}(\psi_1,\eta) = 0\,, \tag{4.208}$$

where η is an arbitrary function satisfying the boundary conditions. This equation is nothing but

$$\int_a^b dx\,\Big((P\,\psi_1')' + Q\,\psi_1 + R_1\,w\,\psi_1\Big)\,\eta = 0\,, \tag{4.209}$$

and if this is to hold for all η, it must be that the integrand vanishes, implying

$$(P\,\psi_1')' + Q\,\psi_1 + R_1\,\omega\,\psi_1 = 0\,. \tag{4.210}$$

In other words, we have learned that the function ψ_1 that minimises the ratio R in (4.195) is precisely an eigenfunction of the Sturm-Liouville equation, $\mathcal{L}\,\psi_1 + R_1\,\omega\,\psi_1 = 0$. Since λ_1 is as small as possible, it follows that ψ_1 is the lowest eigenfunction, and $R_1 = \lambda_1$, the lowest eigenvalue. Let us emphasise also that we now know that for *any* function f that satisfies the boundary conditions, we must have

$$\Omega(f) \ge \lambda_1\,\mathcal{N}(f)\,, \tag{4.211}$$

with equality achieved if and only if f is the lowest eigenfunction.

We now proceed to build the next eigenfunction. We consider the same minimisation problem, but now with the additional constraint that our function f should be orthogonal to ψ_1, i.e. $\mathcal{N}(\psi_1, f) = 0$. In other words, we want to find the next-to-smallest minimum of the ratio R in (4.195), for functions orthogonal to ψ_1. Let us call the solution to this constrained minimisation ψ_2. Thus it will satisfy

$$\Omega(\psi_2) = R_2\,N(\psi_2)\,, \qquad \mathcal{N}(\psi_1,\psi_2) = 0\,. \tag{4.212}$$

Let us emphasise again that we are not yet assuming that ψ_2 is the second eigenfunction, nor that R_2 is the corresponding eigenvalue. We only assume that ψ_2 is the function that minimises $\Omega(f)/\mathcal{N}(f)$, subject to the constraint $\mathcal{N}(\psi_1, f) = 0$.

Now by definition, if we look at $\Omega(\psi_2 + \epsilon\,\eta)$, where ϵ is a constant, and η is an arbitrary function satisfying the boundary conditions, and in addition the constraint

$$N(\psi_1, \eta) = 0\,, \tag{4.213}$$

then by definition we must have

$$\Omega(\psi_2 + \epsilon\,\eta) \ge R_2\, N(\psi_2 + \epsilon\,\eta)\,. \tag{4.214}$$

This is because η is orthogonal to ψ_1, and so adding $\epsilon\,\eta$ to ψ_2 gives precisely a function $f = \psi_2 + \epsilon\,\eta$ that satisfies the constraint $\mathcal{N}(\psi_1, f) = 0$. We agreed that ψ_2 was the solution to this constrained minimisation problem, and so therefore (4.214) must be true.

Now, we can construct η satisfying (4.213) from an arbitrary *unconstrained* function ξ, by writing

$$\eta = \xi - c\,\psi_1\,, \tag{4.215}$$

where

$$c = \frac{\mathcal{N}(\psi_1, \xi)}{\mathcal{N}(\psi_1)}\,. \tag{4.216}$$

(Of course ξ, like every function we ever talk about, will still be assumed to satisfy our Sturm-Liouville boundary conditions.) Thus from (4.214) we will have

$$\Omega(\psi_2 + \epsilon\,\xi - \epsilon\,c\,\psi_1) \ge R_2\,\mathcal{N}(\psi_2 + \epsilon\,\xi - \epsilon\,c\,\psi_1)\,. \tag{4.217}$$

Expanding everything out, we have for $\Omega(\psi_2 + \epsilon\,\xi - \epsilon\,c\,\psi_1)$:

$$\begin{aligned} \Omega(\psi_2 + \epsilon\,\xi - \epsilon\,c\,\psi_1) &= R_2\,\mathcal{N}(\psi_2) + 2\epsilon\,\Omega(\psi_2, \xi) - 2\epsilon\,c\,\Omega(\psi_2, \psi_1) \\ &\quad + \epsilon^2\,\Omega(\xi) + \epsilon^2\,c^2\,\Omega(\psi_1) - 2\epsilon^2\,c\,\Omega(\psi_1, \xi)\,, \\ &= R_2\,\mathcal{N}(\psi_2) + 2\epsilon\,\Omega(\psi_2, \xi) + \epsilon^2\,\Omega(\xi) - \epsilon^2\,c^2\,\lambda_1\,\mathcal{N}(\psi_1)\,. \end{aligned} \tag{4.218}$$

For $\mathcal{N}(\psi_2 + \epsilon\,\xi - \epsilon\,c\,\psi_1)$ we have

$$\begin{aligned} \mathcal{N}(\psi_2 + \epsilon\,\xi - \epsilon\,c\,\psi_1) &= \mathcal{N}(\psi_2) + 2\epsilon\,\mathcal{N}(\psi_2, \xi) - 2\epsilon\,c\,\mathcal{N}(\psi_2, \psi_1) \\ &\quad + \epsilon^2\mathcal{N}(\xi) + \epsilon^2\,c^2\,\mathcal{N}(\psi_1) - 2\epsilon^2\,c\,\mathcal{N}(\psi_1, \xi)\,, \\ &= \mathcal{N}(\psi_2) + 2\epsilon\,\mathcal{N}(\psi_2, \xi) + \epsilon^2\,\mathcal{N}(\xi) - \epsilon^2\,c^2\,\mathcal{N}(\psi_1)\,. \end{aligned} \tag{4.219}$$

In each case, we have made use of previously-derived results in arriving at the second lines. Plugging into (4.217), we thus find that the $O(\epsilon^0)$ terms cancel out, and we are left with

$$2\epsilon\,[\Omega(\psi_2,\xi) - R_2\,\mathcal{N}(\psi_2,\xi)] + \epsilon^2\,[\Omega(\xi) - R_2\,\mathcal{N}(\xi) + (R_2-\lambda_1)\,\mathcal{N}(\psi_1)] \ge 0\,. \qquad (4.220)$$

By the same argument as we used in the original ψ_1 minimisation, this equality can only be true for arbitrary small ϵ if the coefficient of ϵ vanishes:

$$\Omega(\psi_2,\xi) - R_2\,\mathcal{N}(\psi_2,\xi) = 0\,. \qquad (4.221)$$

Since this must hold for all ξ that satisfy the boundary conditions, it follows that like in the previous ψ_1 discussion, here we shall have

$$\mathcal{L}\,\psi_2 + R_2\,w\,\psi_2 = 0\,. \qquad (4.222)$$

So the function that minimises $\Omega(f)/\mathcal{N}(f)$ *subject to the constraint* that it be orthogonal to ψ_1 is an eigenfunction of the Sturm-Liouville equation. By definition, R_2 is the smallest value we can achieve for R in (4.195), for functions f orthogonal to ψ_1. Therefore $R_2 = \lambda_2$, the next-to-smallest eigenvalue.

It should now be evident that we can proceed iteratively in the same manner, to construct all the eigenfunctions and eigenvalues in sequence. At the next step, we consider the constrained minimisation problem where we require that the functions f in $\Omega(f)/\mathcal{N}(f)$ must be orthogonal both to ψ_1 and ψ_2. Following precisely analogous steps to those described above, we then find that the function ψ_3 that achieves the minimum value $R_3 = \lambda_3$ for this ratio is again an eigenfunction of the Sturm-Liouville equation. This will therefore be the third eigenfunction, in the sense $\lambda_1 < \lambda_2 < \lambda_3$.

At the $(N+1)$'th stage in in the process, we look for the function ψ_{N+1} that minimises $R = \Omega(f)/\mathcal{N}(f)$, subject to the requirements that

$$\mathcal{N}(\psi_n, f) = 0\,, \qquad 1 \le n \le N\,. \qquad (4.223)$$

The resulting minimum value for R will be the $(N+1)$'th eigenvalue λ_{N+1}, and ψ_{N+1} will be the $(N+1)$'th eigenfunction.

Let us conclude this part of the discussion by emphasising one important point, which we shall need later. If $f(x)$ is any admissible function that is orthogonal to the first N eigenfunctions, as in (4.223), then it satisfies the inequality

$$\Omega(f) \ge \lambda_{N+1}\,\mathcal{N}(f)\,. \qquad (4.224)$$

Completeness of the Sturm-Liouville Eigenfunctions:

One way to formulate the question of completeness is the following. Suppose we make a partial expansion of the form (4.188), with constant coefficients c_n chosen as in (4.190), but where we run the summation not up to infinity, but instead up to some number N. Obviously we will not in general "hit the target" and get a perfect expansion of the function $f(x)$ like this; at best, we will have some sort of approximation to $f(x)$, which we hope will get better and better as higher and higher modes are included in the sum. In fact we can define

$$f_N(x) \equiv f(x) - \sum_{n=1}^{N} c_n\, u_n(x)\,, \tag{4.225}$$

where the coefficients c_n are defined in (4.190). What we would like to be able to show is that as we send N to infinity, the functions $f_N(x)$, which measure the discrepancy between the true function $f(x)$ and our attempted series expansion, should in some sense tend to zero. The best way to measure this is to define

$$A_N^2 \equiv \int_a^b dx\, w(x)\, (f_N(x))^2 = (f_N, w\, f_N) = \mathcal{N}(f_N)\,. \tag{4.226}$$

Now, if we can show that A_N^2 goes to zero as N goes to infinity, we will be achieving a good least-squares fit.

To show this, we now use the functional $\Omega(f)$ that was defined in (4.191), and the properties that we derived. Before we begin, let us observe that we can, without loss of generality, make the simplifying assumption that $\lambda_1 = 0$. We can do this for the following reason. We know that the eigenvalue spectrum is bounded below, meaning that λ_1, the smallest eigenvalue, must satisfy $\lambda_1 > -\infty$. We can then shift the Sturm-Liouville operator $\mathcal{L}$, defined by $\mathcal{L}u = (P\, u')' + Q\, u$, to $\widetilde{\mathcal{L}} = \mathcal{L} + \lambda_1\, w$, which is achieved by taking $\widetilde{\mathcal{L}}u \equiv (P\, u')' + \widetilde{Q}\, u$, where $\widetilde{Q} = Q + \lambda_1\, w$. Thus we can just as well work with the redefined operator $\widetilde{\mathcal{L}}$, which will therefore have eigenvalues $\tilde{\lambda}_n = \lambda_n - \lambda_1 \ge 0$. The set of eigenfunctions will be identical to before, and we have simply arranged to shift the eigenvalues. Let us assume from now on that we have done this, so we drop the tildes, and simply assume that $\lambda_1 = 0$, and in general $\lambda_n \ge 0$.

Now, we define

$$F_N(x) \equiv \frac{f_N(x)}{A_N}\,. \tag{4.227}$$

From (4.226), it is clear that

$$\mathcal{N}(F_N) = 1\,. \tag{4.228}$$

Now consider $\mathcal{N}(u_n, F_N)$. Using (4.225), we have

$$\begin{aligned}\mathcal{N}(u_n, F_N) &= \frac{1}{A_N}\mathcal{N}(u_n, f) - \frac{1}{A_N}\sum_{m=1}^{N} c_m\,\mathcal{N}(u_n, u_m)\,,\\ &= \frac{1}{A_N}\Big(c_n - \sum_{m=1}^{N} c_m\,\delta_{mn}\Big)\,. \end{aligned} \tag{4.229}$$

The delta function in the second term "clicks" only if n lies within the range of the summation index, and so we get:

$$\begin{aligned} 1 \le n \le N: &\qquad (u_n, w\, F_N) = 0\,,\\ n \ge N+1: &\qquad (u_n, w\, F_N) = \frac{c_n}{A_N}\,. \end{aligned} \tag{4.230}$$

This means that $F_N(x)$ is precisely one of those functions that we examined earlier, which is orthogonal to all of the first N eigenfunctions, and thus satisfies (4.223). Since F_N is normalised, satisfying $\mathcal{N}(F_N) = 1$, it then follows from (4.224) and (4.228) that

$$\Omega(F_N) \ge \lambda_{N+1}\,. \tag{4.231}$$

Now, let us calculate $\Omega(F_N)$ directly. From (4.225) and (4.227), we will get

$$A_N^2\,\Omega(F_N) = \Omega(f) + 2\sum_{m=1}^{N} c_m\,(f, \mathcal{L}\,u_m) - \sum_{m=1}^{N}\sum_{n=0}^{N} c_m\,c_n\,(u_n, \mathcal{L}\,u_m)\,. \tag{4.232}$$

In the last two terms, where we have already integrated by parts, we now use the fact that the u_m are Sturm-Liouville eigenfunctions, and so $\mathcal{L}\,u_m$ can be replaced by $-\lambda_m\,w\,u_m$. Now, from the definition (4.190) of the coefficients c_n, we see that we eventually get

$$A_N^2\,\Omega(F_N) = \Omega(f) - \sum_{n=1}^{N} c_n^2\,\lambda_n\,. \tag{4.233}$$

Since we arranged that the eigenvalues satisfy $\lambda_n \ge 0$, it follows from this equation that

$$A_N^2 \le \frac{\Omega(f)}{\Omega(F_N)}\,. \tag{4.234}$$

But we saw earlier in (4.231), that $\Omega(F_N) \ge \lambda_{N+1}$, so we deduce that

$$A_N^2 \le \frac{\Omega(f)}{\lambda_{N+1}}\,. \tag{4.235}$$

Now, $\Omega(f)$ is just a functional of the original function $f(x)$ that we are trying to expand in an eigenfunction series, so it certainly doesn't depend on N. Furthermore, $\Omega(f)$ is definitely positive, $\Omega(f) > 0$ (except in the special case where $f = c\, u_1$, for which it vanishes). The upshot of all this, then, is that (4.235) is telling us that as we send N to infinity, implying that λ_{N+1} goes to infinity, we will have

$$A_N \longrightarrow 0\,. \tag{4.236}$$

This is what we wanted to show. It means that if we take $N = \infty$ in (4.225), we get an accurate least-squares fit, and we may say that

$$f(x) = \sum_{n=1}^{\infty} c_n\, u_n(x)\,, \tag{4.237}$$

where c_n is given by (4.190). Thus the set of eigenfunctions $u_n(x)$ is complete.

Let us take stock of what has been achieved. We started by supposing that we could expand any admissible function $f(x)$ as an infinite sum over the Sturm-Liouville eigenfunctions $u_n(x)$,

$$f(x) = \sum_{n\ge 1} c_n\, u_n(x)\,. \tag{4.238}$$

Immediately, by calculating $\mathcal{N}(u_m, f)$, and using the orthonormality $\mathcal{N}(u_m, u_n) = \delta_{mn}$ of the u_n, one sees that if such an expansion is valid, then the coefficients c_n will be given by

$$c_n = \mathcal{N}(u_n, f) = \int_a^b dx\, w(x)\, u_n(x)\, f(x)\,. \tag{4.239}$$

The thing that has taken us so long to show is that an expansion of the assumed kind (4.238) really does work. That is to say, we showed, after quite a long chain of arguments, that the set of eigenfunctions u_n really is complete. This is the sort of exercise that one usually tends not to go through, but since eigenfunction expansions play such an important rôle in all kinds of branches of physics (for example, they are heavily used in quantum mechanics), it is worthwhile just for once to see how the completeness is established.

Now that we have established the validity of the expansion (4.238), we can restate the notion of completeness as follows. Take the expression (4.239), and substitute it into (4.238):

$$f(x) = \sum_{n\ge 1} \mathcal{N}(u_n, f)\, u_n(x)\,. \tag{4.240}$$

Making this explicit, we have

$$f(x) = \int_a^b dy\, w(y)\, f(y)\, \sum_{n\ge 1} u_n(x)\, u_n(y)\,, \tag{4.241}$$

where, being physicists, we are allowed to sneak the summation through the integral without too much concern. (It is one of those fine points that strictly speaking ought to be examined carefully, but in the end it turns out to be justified.) What we are seeing in (4.241) is that $\sum_n u_n(x)\, u_n(y)$ is behaving exactly like the Dirac delta function $\delta(x-y)$, which has the defining property that

$$f(x) = \int_a^b dy\, f(y)\, \delta(x-y)\,, \tag{4.242}$$

for all reasonable functions f. So we have

$$\sum_{n\ge 1} w(x)\, u_n(x)\, u_n(y) = \delta(x-y)\,. \tag{4.243}$$

The point about the completeness of the eigenfunctions is that the left-hand side of this expression does indeed share with the Dirac delta function the property that it is able to take any admissible function f and regenerate it as in (4.242); it doesn't "miss" any functions.[13] Thus it is often convenient to take (4.243) as the definition of completeness.

Note that it is sometimes more convenient to think of the weight function $w(x)$ as part of the integration measure, in which case we could define a slightly different delta-function, let us call it $\delta(x,y)$, as

$$\delta(x,y) = \sum_{n\ge 1} u_n(x)\, u_n(y) \tag{4.244}$$

We would then have

$$f(x) = \int_a^b dy\, w(y)\, f(y)\, \delta(x,y)\,. \tag{4.245}$$

Put another way, we would have

$$\delta(x-y) = w(x)\, \delta(x,y)\,. \tag{4.246}$$

The Dirac delta function is an example of what are called *generalised functions*. When Dirac first introduced the delta function, the mathematicians were a bit sniffy about it, since they hadn't thought of them first, complaining that they weren't well-defined, that derivatives of delta functions were even less well-defined, and so on.[14] These were in fact perfectly valid objections to raise, and sorting out the new mathematics involved in making them "respectable" led to the whole subject of generalised functions. However, it is perhaps worth noting that unlike Dirac, who simply went ahead with using them regardless, the mathematicians who sorted out the details never won the Nobel Prize.

[13] We can put either $w(x)$ or $w(y)$ in this expression, since the right-hand side tells us that the function is non-zero only when $x = y$.

[14] It is surprisingly common in research to encounter one or more of the following reactions: (1) "It's wrong;" (2) "It's trivial;" (3) "I did it first." Interestingly, it is not unknown to get all three reactions simultaneously from the same person.

Let us pause here to say a bit more about the delta function. A useful "physical" picture to keep in mind is that the delta function $\delta(x)$ looks like a "spike" at $x = 0$ that is infinitely high, and infinitessimally narrow, such that its total area is unity. Thus we may think of $\delta(x)$ as the limit of a rectangular function defined as follows:

$$\begin{aligned} h(x) &= 0 \quad \text{for} \quad x < -a \quad \text{and} \quad x > +a\,, \\ h(x) &= \frac{1}{2a} \quad \text{for} \quad -a \le x \le a\,. \end{aligned} \tag{4.247}$$

Clearly this function has area $2a \times 1/(2a) = 1$. In the limit where a goes to zero, we obtain the delta function $\delta(x)$. Obviously, we also have $h(x) = h(-x)$. If we consider the integral

$$G(x) = \int_{-\infty}^{\infty} dy\, h(y-x)\, f(y) \tag{4.248}$$

we shall clearly have

$$G(x) = \frac{1}{2a} \int_{x-a}^{x+a} dy\, f(y)\,. \tag{4.249}$$

As the constant a is taken smaller and smaller, the function $f(y)$ inside the integral becomes more and more nearly constant over the ever-narrowing integration range centred on $y = x$. For small enough a, we can therefore to an excellent approximation pull f outside the integral, simply taking it to be $f(x)$. We are left with the integral

$$G(x) \approx \frac{f(x)}{2a} \int_{x-a}^{x+a} dy = f(x)\,. \tag{4.250}$$

By the time a is taken infinitessimally small the approximation has become arbitrarily good, and so in the limit we have

$$\int_{-\infty}^{\infty} dy\, \delta(y-x)\, f(y) = f(x)\,. \tag{4.251}$$

Note that we don't actually need to take the integration range to be the entire real line; as long as it is over an interval that encompasses $x = y$, we shall get the same result.

4.5.5 Eigenfunction expansions for Green functions

Suppose now that we want to solve the inhomogeneous equation

$$\mathcal{L}u(x) + \lambda\, w(x)\, u(x) = f(x)\,, \tag{4.252}$$

where as usual $\mathcal{L}u = (P\,u')' + Q\,u$ is a Sturm-Liouville operator, $w(x)$ is the weight function, and now we have the inhomogeneous source term $f(x)$. Let us assume that for some suitable admissible boundary conditions at a and b, we have eigenfunctions $u_n(x)$ with eigenvalues λ_n for the usual Sturm-Liouville problem:

$$\mathcal{L}u_n + \lambda_n\, w\, u_n = 0\,. \tag{4.253}$$

Now, let us look for a solution $u(x)$ to the inhomogeneous problem (4.252), where we shall assume that $u(x)$ satisfies the same boundary conditions as the eigenfunctions $u_n(x)$. Since $u(x)$ is thus assumed to be an admissible function, it follows from our previous discussion of completeness that we can expand it as

$$u(x) = \sum_{n\ge 1} b_n\, u_n(x)\,, \tag{4.254}$$

for constant coefficients b_n that we shall determine. Plugging this into (4.252), and making use of (4.253) to work out $\mathcal{L}u_n$, we therefore obtain

$$\sum_{n\ge 1} b_n\,(\lambda - \lambda_n)\, w(x)\, u_n(x) = f(x)\,. \tag{4.255}$$

Now multiply this $u_m(x)$ and integrate from a to b. Using the orthogonality of eigenfunctions u_m, we therefore get

$$b_m\,(\lambda - \lambda_m) = \int_a^b dx\, u_m(x)\, f(x)\,. \tag{4.256}$$

Plugging this back into (4.254), we see that we have

$$u(x) = \int_a^b dy\, f(y) \sum_{n\ge 1} \frac{u_n(x)\, u_n(y)}{\lambda - \lambda_n}\,, \tag{4.257}$$

where as usual we exercise our physicist's prerogative of taking summations freely through integrations. Note that we have been careful to distinguish the integration variable y from the free variable x in $u(x)$.

Equation (4.257) is of the form

$$u(x) = \int_a^b dy\, G(x,y)\, f(y)\,, \tag{4.258}$$

with $G(x,y)$ given here by

$$G(x,y) = \sum_{n\ge 1} \frac{u_n(x)\, u_n(y)}{\lambda - \lambda_n}\,. \tag{4.259}$$

The quantity $G(x,y)$ is known as the *Green Function* for the problem; it is precisely the kernel which allows one to solve the inhomogeneous equation by integrating it times the source term, as in (4.258).[15]

We may note the following properties of the Green function. First of all, from (4.259), we see that it is symmetric in its two arguments,

$$G(x,y) = G(y,x)\,. \tag{4.260}$$

Secondly, since by construction the function $u(x)$ in (4.258) must satisfy (4.252), we may substitute in to find what equation $G(x,y)$ must satisfy. Doing this, we get

$$\mathcal{L}u + \lambda\, w\, u = \int_a^b dy\, (\mathcal{L} + \lambda\, w)\, G(x,y)\, f(y) = f(x)\,, \tag{4.261}$$

where it is understood that the functions P, Q and w depend on x, not y, and that the derivatives in $\mathcal{L}$ are with respect to x. Since the second equality here must hold for any $f(x)$, it follows that the quantity multiplying $f(y)$ in the integral must be precisely the Dirac delta function, and so it must be that

$$\mathcal{L}\, G(x,y) + \lambda\, w\, G(x,y) = \delta(x-y)\,, \tag{4.262}$$

again with the understanding that $\mathcal{L}$ and w depend on x.

We can test directly that our expression (4.259) for $G(x,y)$ indeed satisfies (4.262). Substituting it in, and making use of the fact that the eigenfunctions u_n satisfy (4.253), we see that we get

$$\mathcal{L}\, G(x,y) + \lambda\, w\, G(x,y) = \sum_{n\ge 1} w(x)\, u_n(x)\, u_n(y)\,. \tag{4.263}$$

But this is precisely the expression for $\delta(x-y)$ that we obtained in (4.243).

There are interesting, and sometimes useful, consequences of the fact that we can express the Green function in the form (4.259). Recall that the constant λ in (4.259) is just a parameter that appeared in the original inhomogeneous equation (4.252) that we are solving. It has nothing directly to do with the eigenvalues λ_n arising in the Sturm-Liouville problem (4.253). However, it is clear from the expression (4.259) that there will be a divergence, i.e.

[15] A little digression on English usage is unavoidable here. Contrary to what one might think from the way many physicists and mathematicians write (including, regrettably, in the A&M Graduate Course Catalogue), these functions are named after George Green, who was an English mathematician (1793-1841); he was not called George Greens, nor indeed George Green's. Consequently, they should be called *Green Functions*, and not *Green's Functions*. It would be no more proper to speak of "a Green's function" than it would to speak of "a Legendre's polynomial," or "a Fermi's surface" or "a Lorentz's transformation" or "a Taylor's series" or "the Dirac's equation" or "the quantum Hall's effect." By contrast, another common error (also to be seen in the Graduate Course Catalogue) is to speak of "the Peierl's Instability" in condensed matter physics. The relevant person here is Rudolf Peierls, not Rudolf Peierl's or Rudolf Peierl.

pole, in the expression for $G(x,y)$ whenever λ is chosen to be equal to any of the Sturm-Liouville eigenvalues λ_n. It is a bit like a "resonance" phenomenon, where the solution of a forced harmonic oscillator equation goes berserk if the source term (the forcing function) is chosen to be oscillatory with the natural period of oscillation of the homogeneous (unforced) equation.

Here, what is happening is that if the constant λ is chosen to be equal to one of the Sturm-Liouville eigenvalues, say $\lambda = \lambda_N$, then we suddenly find that we are free to add in a constant multiple of the corresponding eigenfunction $u_N(x)$ to our inhomogeneous solution, since $u_N(x)$ now happens to be precisely the solution of the homogeneous equation $\mathcal{L}u + \lambda\, w\, u = 0$. (For generic λ, none of the eigenfunctions $u_n(x)$ solves the homogeneous equation.) The divergence in the Green function is arising because suddenly that particular eigenfunction $u_N(x)$ is playing a dominant rôle in the eigenfunction expansion for the solution.

Recall now that some lectures ago we actually encountered another way of constructing the Green function for this problem, although we didn't call it that at the time. In (4.45) we obtained a solution to the inhomogeneous second-order ODE, in a form that translates, in our present case, to

$$u(x) = y_2(x) \int_{x_1}^{x} dt\, f(t) \frac{y_1(t)}{\Delta(y_1, y_2)(t)} - y_1(x) \int_{x_2}^{x} dt\, f(t) \frac{y_2(t)}{\Delta(y_1, y_2)(t)} - \,, \tag{4.264}$$

where y_1 and y_2 are the two solutions of the homogeneous equation, which for us will be $\mathcal{L}y + \lambda\, w\, y = 0$, and $\Delta(y_1, y_2)(t) = y_1(t)\, y_2'(t) - y_2(t)\, y_1'(t)$ is the Wronskian of the two solutions. Recall that taking different choices for the lower limits of integration x_1 and x_2 just corresponds to adding different constant multiples of the two solutions of the homogeneous equation. Thus the choices of x_1 and x_2 parameterise the most general solution of the inhomogeneous equation. This freedom is used in order to fit the boundary conditions we wish to impose on $u(x)$.

Suppose, as an example, that our boundary conditions are $u(a) = 0 = u(b)$. We may, for convenience, choose to specify the homogeneous solutions $y_1(x)$ and $y_2(x)$ by requiring[16]

$$y_1(a) = 0\,, \qquad y_2(b) = 0\,. \tag{4.265}$$

This choice is not obligatory; *any* choice of boundary conditions for $y_1(x)$ and $y_2(x)$ will allow us to solve the inhomogeneous equation, as long as we make sure that our boundary conditions lead to linearly-independent solutions $y_1(x)$ and $y_2(x)$. (We know this because we have already proved that (4.264) gives the most general possible solution of the inhomogeneous solution, provided that y_1 and y_2 are linearly-independent solutions of the homogeneous equation.) The choice in (4.265) is very convenient, as we shall now see.

In our example, we want our inhomogeneous solution $u(x)$ to satisfy $u(a) = 0$ and $u(b) = 0$. To ensure these two conitions, we have at our disposal to choose the two integration limits x_1 and x_2. In view of (4.265), we can see that $u(a) = 0$ implies we should take $x_1 = a$. Similarly, $u(b) = 0$ implies we should take $x_2 = b$. Thus from (4.264) we can write the solution as

$$u(x) = \int_a^x dt\, f(t) \frac{y_1(t)\, y_2(x)}{\Delta(y_1, y_2)} + \int_x^b dt\, f(t)\, \frac{y_2(t)\, y_1(x)}{\Delta(y_1, y_2)}\,, \tag{4.266}$$

(Note that the sign has changed on the second term because we have reversed the order of the limits.)

Note that (4.266) can be interpreted as the equation

$$u(x) = \int_a^b dt\, G(x,t)\, f(t)\,, \tag{4.267}$$

where the Green function $G(x,t)$ is given by

$$\begin{aligned} G(x,t) &= \frac{y_1(x)\, y_2(t)}{\Delta(y_1, y_2)} \qquad \text{if } x \le t\,, \\ &= \frac{y_2(x)\, y_1(t)}{\Delta(y_1, y_2)} \qquad \text{if } x \ge t\,. \end{aligned} \tag{4.268}$$

Here $\Delta(y_1, y_2)$ is a function of the integration variable, t.

We can now try comparing this result with our previous eigenfunction expansion (4.259) for the Green function, since the two should in principle agree. Doing this in general would

[16] A full specification of boundary conditions that leads to a unique solution requires *two* conditions, and not just one. For example, $y_1(x)$ is not fully pinned down simply by specifiying $y_1(a) = 0$, since we can take any constant multiple of $y_1(x)$ and it again satisfies the condition of vanishing at $x = a$. But this scaling arbitrariness is completely unimportant in the present context, because, as can be seen from (4.264), y_1 appears linearly in both the numerator and the denominator (via the Wronskian) in each term, as does y_2. Thus we do not need to specify the scale factor in y_1 and y_2, and so we need only specify the one condition on each of y_1 and y_2.

be difficult, since one is an infinite sum and the other is not. Let us consider a simple example, and just compare some of the key features. Take the case that we looked at earlier, where

$$\mathcal{L} = \frac{d^2}{dx^2}\,, \qquad w(x) = 1\,. \tag{4.269}$$

Let us choose our boundaries to be at $a = 0$ and $b = \pi$, at which points we require our eigenfunctions to vanish. We also seek a solution of the inhomogeneous equation

$$\frac{d^2 u(x)}{dx^2} + \lambda\, u(x) = f(x) \tag{4.270}$$

for which $u(0) = u(\pi) = 0$. We saw before that the eigenfunctions and eigenvalues for the Sturm-Liouville problem

$$u_n'' + \lambda_n\, u_n = 0 \tag{4.271}$$

will be

$$u_n(x) = \sqrt{\frac{2}{\pi}}\, \sin nx\,, \qquad \lambda_n = n^2\,, \tag{4.272}$$

for the positive integers n. (We didn't give the normalisation before.) Thus from (4.259) the Green function for the inhomogeneous problem is

$$G(x,t) = \frac{2}{\pi} \sum_{n\ge 1} \frac{\sin nx\, \sin nt}{\lambda - n^2}\,. \tag{4.273}$$

On the other hand, for the closed-form expression (4.268), the required solutions of the homogeneous equation $y'' + \lambda\, y = 0$, such that $y_1(0) = 0$ and $y_2(\pi) = 0$ are (choosing the scale factors to be 1 for simplicity)

$$y_1(x) = \sin(\lambda^{\frac12}\, x)\,, \qquad y_2(x) = \sin(\lambda^{\frac12}\,(x-\pi))\,. \tag{4.274}$$

From these, the Wronskian is easily found:

$$\begin{aligned} \Delta(y_1,y_2) &= \lambda^{\frac12}\Big[\sin(\lambda^{\frac12}\, x)\, \cos(\lambda^{\frac12}\,(x-\pi)) - \cos(\lambda^{\frac12}\, x)\, \sin(\lambda^{\frac12}\,(x-\pi))\Big]\,, \\ &= \lambda^{\frac12}\, \sin(\lambda^{\frac12}\, \pi)\,. \end{aligned} \tag{4.275}$$

We should be able to see the same resonance phenomenon of which we spoke earlier, in both of the (equivalent) expressions for the Green function. In (4.273), we clearly see a resonance whenever λ is equal to the square of an integer, $\lambda = N^2$. On the other hand, in the closed-form expression (4.268), we can see in this case that the only divergences can possibly come from the Wronskian in the denominator, since y_1 and y_2 themselves are just sine functions. Sure enough, we see from (4.275) that the Wronskian vanishes if $\lambda^{\frac12}\, \pi = N\, \pi$, or, in other words, at $\lambda = N^2$. So indeed the pole structure of the Green function is the same in the two expressions.

5 Functions of a Complex Variable

5.1 Complex Numbers, Quaternions and Octonions

The extension from the real number system to complex numbers is an important one both within mathematics itself, and also in physics. The most obvious area of physics where they are indispensable is quantum mechanics, where the wave function is an intrinsically complex object. In mathematics their use is very widespread. One very important point is that by generalising from the real to the complex numbers, it becomes possible to treat the solution of polynomial equations in a uniform manner, since now not only equations like $x^2 - 1 = 0$ but also $x^2 + 1 = 0$ can be solved.

The complex numbers can be defined in terms of ordered pairs of real numbers. Thus we may *define* the complex number z to be the ordered pair $z = (x, y)$, where x and y are real. Of course this doesn't tell us much until we give some rules for how these quantities behave. First, we may define $(x, 0)$ to be an ordinary real number, so that we may take

$$(x, 0) \sim x\,. \tag{5.1}$$

If $z = (x, y)$, and $z' = (x', y')$ are two complex numbers, and a is any real number, then the rules can be stated as

$$\begin{aligned} z + z' &= (x + x', y + y')\,, \\ a\,z &= (a\,x, a\,y)\,, \\ z\,z' &= (x\,x' - y\,y', x\,y' + x'\,y)\,. \end{aligned} \tag{5.2}$$

We also define the *complex conjugate* of $z = (x, y)$, denoted by $\bar{z}$, as

$$\bar{z} = (x, -y)\,. \tag{5.3}$$

and the *modulus* of z, denoted by $|z|$, as the positive square root of $|z|^2$ defined by

$$|z|^2 = \bar{z}\,z = (x^2 + y^2, 0) = x^2 + y^2\,. \tag{5.4}$$

It is manifest that $|z| \ge 0$, with $|z| = 0$ if and only if $z = 0$.

It is now straightforward to verify that the following fundamental laws of algebra are satisfied:

1. *Commutative and Associative Laws of Addition*:

$$\begin{aligned} z_1 + z_2 &= z_2 + z_1\,, \\ z_1 + (z_2 + z_3) &= (z_1 + z_2) + z_3 = z_1 + z_2 + z_3\,, \end{aligned} \tag{5.5}$$

2. *Commutative and Associative Laws of Multiplication*:

$$\begin{aligned} z_1\, z_2 &= z_2\, z_1\,, \\ z_1\,(z_2\, z_3) &= (z_1\, z_2)\, z_3 = z_1\, z_2\, z_3\,, \end{aligned} \tag{5.6}$$

3. *Distributive Law*:

$$(z_1 + z_2)\, z_3 = z_1\, z_3 + z_2\, z_3\,. \tag{5.7}$$

We can also define the operation of division. If $z_1\, z_2 = z_3$, then we see from the previous rules that, multiplying by $\bar{z}_1$, we have

$$\bar{z}_1\,(z_1\, z_2) = (\bar{z}_1\, z_1)\, z_2 = |z_1|^2\, z_2 = \bar{z}_1\, z_3\,, \tag{5.8}$$

and so, provided that $|z_1| \neq 0$, we can write the *quotient*

$$z_2 = \frac{z_3\, \bar{z}_1}{|z_1|^2} = \frac{z_3}{z_1}\,. \tag{5.9}$$

(The expression $z_3\, \bar{z}_1/|z_1|^2$ here defines what we mean by z_3/z_1.)

We can, of course, recognise that from the previous rules we have that the square of the complex number $(0,1)$ is $(-1,0)$, which we agreed to call simply -1. Thus we can view $(0,1)$ as being the square root of -1:

$$(0,1) \sim \mathrm{i} = \sqrt{-1}\,. \tag{5.10}$$

We can now use the familiar abbreviated notation for complex numbers

$$z = x + \mathrm{i}\, y\,. \tag{5.11}$$

The symbol i is called the *imaginary unit.*

One might be wondering at this stage what all the fuss is about; we appear to be making rather a meal out of saying some things that are pretty obvious. Well, one reason for this is that one can also go on to consider more general types of "number fields," in which some of the previous properties cease to hold. It then becomes very important to formalise things properly, so that there is a clear set of statements of what is true and what is not. For example, the "next" extension beyond the complex numbers is to the *quaternions*, where one has three independent imaginary units, usually denoted by i, j and k, subject to the rules

$$\mathrm{i}^2 = \mathrm{j}^2 = \mathrm{k}^2 = -1\,, \qquad \mathrm{i}\,\mathrm{j} = -\mathrm{j}\,\mathrm{i} = \mathrm{k}\,, \qquad \mathrm{j}\,\mathrm{k} = -\mathrm{k}\,\mathrm{j} = \mathrm{i}\,, \qquad \mathrm{k}\,\mathrm{i} = -\mathrm{i}\,\mathrm{k} = \mathrm{j}\,. \tag{5.12}$$

A quaternion q is then a quantity of the form

$$q = q_0 + q_1 \, \mathrm{i} + q_2 \, \mathrm{j} + q_3 \, \mathrm{k} \,, \tag{5.13}$$

where q_0, q_1, q_2 and q_3 are all real numbers. There is again an operation of complex conjugation, $\bar{q}$, in which the signs of all three of i, j and k are reversed

$$\bar{q} = q_0 - q_1 \, \mathrm{i} - q_2 \, \mathrm{j} - q_3 \, \mathrm{k} \,, \tag{5.14}$$

The modulus $|q|$ of a quaternion q is a real number, defined to be the positive square root of

$$|q|^2 \equiv \bar{q} \, q = q \, \bar{q} = q_0^2 + q_1^2 + q_2^2 + q_3^2 \,. \tag{5.15}$$

Clearly $|q| \ge 0$, with equality if and only if $q = 0$.

Which of the previously-stated properties of complex numbers still hold for the quaternions? It is not so obvious, until one goes through and checks. It is perfectly easy to do this, of course; the point is, though, that it does now need a bit of careful checking, and the value of setting up a formalised structure that defines the rules becomes apparent. The answer is that for the quaternions, one has now lost multiplicative commutativity, so $q \, q' \ne q' \, q$ in general. A consequence of this is that there is no longer a unique definition of the quotient of quaternions. However, a very important point is that we *do* keep the following property. If q and q' are two quaternions, then we have

$$|q \, q'| = |q| \, |q'| \,, \tag{5.16}$$

as one can easily verify from the previous definitions.

Let us note that for the quaternions, if we introduce the notation γ_a for $a = 1, 2, 3$ by

$$\gamma_1 = \mathrm{i} \,, \qquad \gamma_2 = \mathrm{j} \,, \qquad \gamma_3 = \mathrm{k} \,, \tag{5.17}$$

then the algebra of the quaternions, given in (5.12), can be written as

$$\gamma_a \, \gamma_b = -\delta_{ab} + \epsilon_{abc} \, \gamma_c \,, \tag{5.18}$$

where ϵ_{abc} is the totally antisymmetric tensor with

$$\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1 \,, \quad \epsilon_{132} = \epsilon_{321} = \epsilon 213 = -1 \,. \tag{5.19}$$

Note that the Einstein summation convention for the repeated c index is understood, so (5.18) really means

$$\gamma_a \, \gamma_b = -\delta_{ab} + \sum_{c=1}^{3} \epsilon_{abc} \, \gamma_c \,. \tag{5.20}$$

In fact, one can recognise this as the multiplication algebra of $-\sqrt{-1}$ times the Pauli matrices σ_a of quantum mechanics, $\gamma_a = -\sqrt{-1}\,\sigma_a$, which can be represented as

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -\sqrt{-1} \\ \sqrt{-1} & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.21}$$

(We use the rather clumsy notation $\sqrt{-1}$ here to distinguish this "ordinary" square root of minus one from the i quaternion.) In this representation, the quaternion defined in (5.13) is therefore written as

$$q = \begin{pmatrix} q_0 - \sqrt{-1}\,q_3 & -\sqrt{-1}\,q_1 - q_2 \\ -\sqrt{-1}\,q_1 + q_2 & q_0 + \sqrt{-1}\,q_3 \end{pmatrix}. \tag{5.22}$$

Since the quaternions are now represented by matrices, it is immediately clear that we shall have associativity, $A(BC) = (AB)C$, but not commutativity, under multiplication.

As a final remark about the quaternions, note that we can define them as an ordered pair of complex numbers. Thus we may define

$$q = (a, b) = a + b\,\mathrm{j} = a_0 + a_1\,\mathrm{i} + b_0\,\mathrm{j} + b_1\,\mathrm{k}\,, \tag{5.23}$$

where $a = a_0 + a_1\,\mathrm{i}$, $b = b_0 + b_1\,\mathrm{i}$. Here, we assign to i and j the multiplication rules given in (5.12), and k is, by definition, nothing but $\mathrm{i}\,\mathrm{j}$. Quaternionic conjugation is given by $\bar{q} = (\bar{a}, -b)$. The multiplication rule for the quaternions $q = (a, b)$ and $q' = (c, d)$ can then easily be seen to be

$$q\,q' = (a\,c - b\,\bar{d}, a\,d + b\,\bar{c})\,. \tag{5.24}$$

To see this, we just expand out $(a + b\,\mathrm{j})(c + d\,\mathrm{j})$:

$$\begin{aligned} (a + b\,\mathrm{j})(c + d\,\mathrm{j}) &= a\,c + b\,\mathrm{j}\,d\,\mathrm{j} + a\,d\,\mathrm{j} + b\,\mathrm{j}\,c \\ &= a\,c + b\,\bar{d}\,\mathrm{j}^2 + a\,d\,\mathrm{j} + b\,\bar{c}\,\mathrm{j} \\ &= (a\,c - b\,\bar{d}) + (a\,d + b\,\bar{c})\,\mathrm{j} \\ &= (a\,c - b\,\bar{d}, a\,d + b\,\bar{c})\,. \end{aligned} \tag{5.25}$$

Note that the complex conjugations in this expression arise from taking the quaternion j through the quaternion i, which generates a minus sign, thus

$$\begin{aligned} \mathrm{j}\,c &= \mathrm{j}\,(c_0 + c_1\,\mathrm{i}) = c_0\,\mathrm{j} + c_1\,\mathrm{j}\,\mathrm{i} \\ &= c_0\,\mathrm{j} - c_1\,\mathrm{i}\,\mathrm{j} = (c_0 - c_1\,\mathrm{i})\,\mathrm{j} = \bar{c}\,\mathrm{j}\,. \end{aligned} \tag{5.26}$$

Notice that the way quaternions are defined here as ordered pairs of complex numbers is closely analogous to the definition of the complex numbers themselves as ordered pairs of real numbers. The multiplication rule (5.24) is also very like the multiplication rule in the last line in (5.2) for the complex numbers. Indeed, the only real difference is that for the quaternions, the notion of complex conjugation of the constituent complex numbers arises. It is because of this that commutativity of the quaternions is lost.

The next stage after the quaternions is the *octonions*, where one has 7 independent imaginary units. The rules for how these combine is quite intricate, leading to the rather splendidly-named *Zorn Product* between two octonions. It turns out that for the octonions, not only does one not have multiplicative commutativity, but multiplicative associativity is also lost, meaning that $A\,(B\,C) \neq (A\,B)\,C$ in general.

For the octonions, let us denote the 7 imaginary units by γ_a, where now $1 \le a \le 7$. Their multiplication rule is reminiscent of (5.18), but instead is

$$\gamma_a\,\gamma_b = -\delta_{ab} + c_{abc}\,\gamma_c\,, \tag{5.27}$$

where c_{abc} are a set of *totally-antisymmetric* constant coefficients, and the Einstein summation convention is in operation, meaning that the index c in the last term is understood to be summed over the range 1 to 7. Note that the total antisymmetry of c_{abc} means that the interchange of *any* pair of indices causes a sign change; for example, $c_{abc} = -c_{bac}$. A convenient choice for the c_{abc}, which are known as the *structure constants* of the octonion algebra, is

$$c_{147} = c_{257} = c_{367} = c_{156} = c_{264} = c_{345} = -1\,, \qquad c_{123} = +1\,. \tag{5.28}$$

Here, it is to be understood that all components related to these by the antisymmetry of c_{abc} will take the values implied by the antisymmetry, while all other components not yet specified are zero. For example, we have $c_{174} = +1$, $c_{321} = -1$, $c_{137} = 0$.

We may think of an octonion w as an object built from 8 real numbers w_0 and w_a, with

$$w = w_0 + w_a\,\gamma_a\,. \tag{5.29}$$

There is a notion of an *octonionic conjugate*, where the signs of the 7 imaginary units are reversed:

$$\bar w = w_0 - w_a\,\gamma_a\,, \tag{5.30}$$

and there is a modulus $|w|$, which is a real number defined by

$$|w|^2 \equiv \bar w\, w = w_0^2 + \sum_{a=1}^{7} w_a^2\,. \tag{5.31}$$

Note that $|w| \ge 0$, and $|w|$ vanishes if and only if $w = 0$.

One can verify from (5.28) that

$$c_{abc}\, c_{ade} = \delta_{bd}\, \delta_{ce} - \delta_{be}\, \delta_{cd} - c_{bcde}\,, \tag{5.32}$$

where an absolutely crucial point is that c_{bcde} is also *totally antisymmetric*. In fact,

$$c_{bcde} = \tfrac{1}{6} \epsilon_{bcdefgh}\, c_{fgh}\,, \tag{5.33}$$

where $\epsilon_{bcdefgh}$ is the totally-antisymmetric tensor of 7 dimensions, with $\epsilon_{1234567} = +1$.

It is straightforward to see that the octonions are non-associative. For example, from the rules given above we can see that

$$\gamma_3\, (\gamma_1\, \gamma_7) = \gamma_3\, c_{174}\, \gamma_4 = \gamma_3\, \gamma_4 = c_{345}\, \gamma_5 = -\gamma_5\,, \tag{5.34}$$

whilst

$$(\gamma_3\, \gamma_1)\, \gamma_7 = c_{312}\, \gamma_2\, \gamma_7 = \gamma_2\, \gamma_7 = c_{275}\, \gamma_5 = +\gamma_5\,. \tag{5.35}$$

So what *does* survive? An important thing that is still true for the octonions is that any two of them, say w and w', will satisfy

$$|w\, w'| = |w|\, |w'|\,. \tag{5.36}$$

Most importantly, all of the real, complex, quaternionic and octonionic algebras are *division algebras*. This means that the concept of division makes sense, which is perhaps quite surprising in the case of the octonions. Suppose that A, B and C are any three numbers in any one of these four number systems. First note that we have

$$\bar{A}\, (A\, B) = (\bar{A}\, A)\, B\,. \tag{5.37}$$

This is obvious from the associativity for the real, complex or quaternionic algebras. It is not obvious for the octonions, since they are not associative (i.e. $A\, (B\, C) \neq (A\, B)\, C$), but a straightforward calculation using the previously-given properties shows that it is true for the special case $\bar{A}\, (A\, B) = (\bar{A}\, A)\, B$. Thus we can consider the following manipulation. If $A\, B = C$, then we will have

$$\bar{A}\, (A\, B) = |A|^2\, B = \bar{A}\, C\,. \tag{5.38}$$

Hence we have

$$B = \frac{\bar{A}\, C}{|A|^2}\,, \tag{5.39}$$

where we are allowed to divide by the real number $|A|^2$, provided that it doesn't vanish. Thus as long as $A \neq 0$, we can give meaning to the division of C by A. This shows that all four of the number systems are division algebras.

Finally, note that again we can define the octonions as an ordered pair of the previous objects, i.e. quaternions, in this chain of real, complex, quaternionic and octonionic division algebras. Thus we define the octonion $w = (a, b) = a + b\,\gamma_7$, where $a = a_0 + a_1\,\mathrm{i} + a_2\,\mathrm{j} + a_3\,\mathrm{k}$ and $b = b_0 + b_1\,\mathrm{i} + b_2\,\mathrm{j} + b_3\,\mathrm{k}$ are quaternions, and $\mathrm{i} = \gamma_1$, $\mathrm{j} = \gamma_2$ and $\mathrm{k} = \gamma_3$. The conjugate of w is given by $\bar{w} = (\bar{a}, -b)$. It is straightforward to show, from the previously-given multiplication rules for the imaginary octonions, that the rule for multiplying octonions $w = (a, b)$ and $w' = (c, d)$ is

$$w\,w' = (a\,c - \bar{d}\,b, d\,a + b\,\bar{c})\,. \tag{5.40}$$

This is very analogous to the previous multiplication rule (5.24) that we found for the quaternions. Note, however, that the issue of ordering of the constituent quaternions in these octonionic products is now important, and indeed a careful calculation from the multiplication rules shows that the ordering must be as in (5.40). In fact (5.40) is rather general, and encompasses all three of the multiplication rules that we have met. As a rule for the quaternions, the ordering of the complex-number constituents in (5.40) would be unimportant, and as a rule for the complex numbers, not only the ordering but also the complex conjugation of the real-number constituents would be unimportant.

After discussing the generalities of division algebras, let us return now to the complex numbers, which is the subject we wish to develop further here. Since a complex number z is an ordered pair of real numbers, $z = (x, y)$, it is natural to represent it as a point in the two-dimensional plane, whose Cartesian axes are simply x and y. This is known as the *Complex Plane*, or sometimes the *Argand Diagram*. Of course it is also often convenient to employ polar coordinates r and θ in the plane, related to the Cartesian coordinates by

$$x = r\,\cos\theta\,, \qquad y = r\,\sin\theta\,. \tag{5.41}$$

Since we can also write $z = x + \mathrm{i}\,y$, we therefore have

$$z = r\,(\cos\theta + \mathrm{i}\,\sin\theta)\,. \tag{5.42}$$

Note that $|z|^2 = r^2\,(\cos^2\theta + \sin^2\theta) = r^2$.

Recalling that the power-series expansions of the exponential function, the cosine and the sine functions are given by

$$e^x = \sum_{n\ge 0} \frac{x^n}{n!}\,, \qquad \cos x = \sum_{p\ge 0} \frac{(-1)^p\,x^{2p}}{(2p)!}\,, \qquad \sin x = \sum_{p\ge 0} \frac{(-1)^p\,x^{2p+1}}{(2p+1)!}\,, \tag{5.43}$$

we can see that in particular, in the power series expansion of $e^{\mathrm{i}\,\theta}$ the real terms (even powers of θ assemble into the power series for $\cos\theta$, whilst the imaginary terms (odd powers of θ) assemble into the series for $\sin\theta$. In other words

$$e^{\mathrm{i}\,\theta} = \cos\theta + \mathrm{i}\,\sin\theta\,. \tag{5.44}$$

Turning this around, which can be achieved by adding or subtracting the comlex conjugate, we find

$$\cos\theta = \tfrac{1}{2}(e^{\mathrm{i}\,\theta} + e^{-\mathrm{i}\,\theta})\,, \qquad \sin\theta = \tfrac{1}{2\mathrm{i}}(e^{\mathrm{i}\,\theta} - e^{-\mathrm{i}\,\theta})\,. \tag{5.45}$$

Combining (5.42) and (5.44), we therefore have

$$z = r\,e^{\mathrm{i}\,\theta}\,. \tag{5.46}$$

Note that we can also write this as $z = |z|\,e^{\mathrm{i}\,\theta}$. The angle θ is known as the *phase*, or the *argument*, of the complex number z. When complex numbers are multiplied together, the phases are additive, and so if $z_1 = |z_1|\,e^{\mathrm{i}\,\theta_1}$ and $z_2 = |z_2|\,e^{\mathrm{i}\,\theta_2}$, then

$$z_1\,z_2 = |z_1|\,|z_2|\,e^{\mathrm{i}\,(\theta_1+\theta_2)}\,. \tag{5.47}$$

We may note that the following inequality holds:

$$|z_1 + z_2| \le |z_1| + |z_2|\,. \tag{5.48}$$

This can be seen by calculating the square:

$$\begin{aligned} |z_1+z_2|^2 &= (\bar z_1 + \bar z_2)(z_1+z_2) = |z_1|^2 + |z_2|^2 + \bar z_1\,z_2 + \bar z_2\,z_1\,, \\ &= |z_1|^2 + |z_2|^2 + 2|z_1\,|z_2|\,\cos(\theta_1-\theta_2)\,, \\ &\le |z_1|^2 + |z_2|^2 + 2|z_1\,|z_2| = (|z_1|+|z_2|)^2\,, \end{aligned} \tag{5.49}$$

where we write $z_1 = |z_1|\,e^{\mathrm{i}\theta_1}$ and $z_2 = |z_2|\,e^{\mathrm{i}\theta_2}$. (The inequality follows from the fact that $\cos\theta \le 1$.) By induction, the inequality (5.48) extends to any finite number of terms:

$$|z_1 + z_2 + \cdots + z_n| \le |z_1| + |z_2| + \cdots + |z_n|\,. \tag{5.50}$$

5.2 Analytic or Holomorphic Functions

Having introduced the notion of complex numbers, we can now consider situations where we have a complex function depending on a complex argument. The most general kind of possibility would be to consider a complex function $f = u + \mathrm{i}\, v$, where u and v are themselves real functions of the complex variable $z = x + \mathrm{i}\, y$;

$$f(z) = u(x, y) + \mathrm{i}\, v(x, y)\,. \tag{5.51}$$

As it stands, this notion of a function of a complex variable is too broad, and consequently of limited value. If functions are to be at all interesting, we must be able to differentiate them. Suppose the function $f(z)$ is defined in some region, or domain, D in the complex plane (the two-dimensional plane with Cartesian axes x and y). We would naturally define the derivative of f at a point z_0 in D as the limit of

$$\frac{f(z) - f(z_0)}{z - z_0} = \frac{\delta f}{\delta z} \tag{5.52}$$

as z approaches z_0. The key point here, though, is that in order to be able to say "the limit," we must insist that the answer is independent of how we let z approach the point z_0. The complex plane, being 2-dimensional, allows z to approach z_0 on any of an infinity of different trajectories. We would like the answer to be unique.

A classic example of a function of z whose derivative is not unique is $f(z) = |z|^2 = \bar{z}\, z$. Thus from (5.52) we would attempt to calculate the limit

$$\frac{|z|^2 - |z_0|^2}{z - z_0} = \frac{z\, \bar{z} - z_0\, \bar{z}_0}{z - z_0} = \bar{z} + z_0 \frac{\bar{z} - \bar{z}_0}{z - z_0}\,. \tag{5.53}$$

Now, if we write $z - z_0 = |z - z_0|\, e^{\mathrm{i}\,\theta}$, we see that this becomes

$$\bar{z} + z_0\, e^{-2\mathrm{i}\,\theta} = \bar{z} + z_0\, (\cos 2\theta - \mathrm{i}\, \sin 2\theta)\,, \tag{5.54}$$

which shows that, except at $z_0 = 0$, the answer depends on the angle θ at which z approaches z_0 in the complex plane. One say that the function $|z|^2$ is not *differentiable* except at $z = 0$.

The interesting functions $f(z)$ to consider are those which *are* differentiable in some domain D in the complex plane. Placing the additional requirement that $f(z)$ be *single valued* in the domain, we have the definition of an *analytic* function, sometimes known as a *holomorphic* function. Thus:

A function $f(z)$ is analytic or holomorphic in a domain D in the complex plane if it is single-valued and differentiable everywhere in D.

Let us look at the conditions under which a function is analytic in D. It is easy to derive *necessary* conditions. Suppose first we take the limit in (5.52) in which $z + \delta z$ approaches z along the direction of the real axis (the x axis), so that $\delta z = \delta x$;

$$\frac{\delta f}{\delta z} = \frac{\delta u + \mathrm{i}\, \delta}{\delta x + \mathrm{i}\, \delta y} = \frac{u_x\, \delta x + \mathrm{i}\, v_x\, \delta x}{\delta x} = u_x + \mathrm{i}\, v_x\,. \tag{5.55}$$

(Clearly for this to be well-defined the partial derivatives $u_x \equiv \partial u/\partial x$ and $v_x \equiv \partial v/\partial x$ must exist.)

Now suppose instead we approach along the imaginary axis, $\delta z = \mathrm{i}\,\delta y$ so that now

$$\frac{\delta f}{\delta z} = \frac{\delta u + \mathrm{i}\,\delta}{\delta x + \mathrm{i}\,\delta y} = \frac{u_y\,\delta y + \mathrm{i}\,v_y\,\delta y}{\mathrm{i}\,\delta y} = -\mathrm{i}\,u_y + v_y\,. \tag{5.56}$$

(This time, we require that the partial derivatives u_y and v_y exist.) If this is to agree with the previous result from approaching along x, we must have $u_x + \mathrm{i}\,v_x = v_y - \mathrm{i}\,u_y$, which, equating real and imaginary parts, gives

$$u_x = v_y\,, \qquad u_y = -v_x\,. \tag{5.57}$$

These conditions are known as the *Cauchy-Riemann equations*. It is quite easy to show that we would derive the same conditions if we allowed δz to lie along any ray that approaches z at any angle.

The Cauchy-Riemann equations by themselves are *necessary* but not *sufficient* for the analyticity of the function f. The full statement is the following:

A continuous single-valued function $f(z)$ is analytic or holomorphic in a domain D if the four derivatives u_x, u_y, v_x and v_y exist, are continuous and satisfy the Cauchy-Riemann equations.[17]

There is a nice alternative way to view the Cauchy-Riemann equations. Since $z = x + \mathrm{i}\,y$, and hence $\bar z = x - \mathrm{i}\,y$, we may solve to express x and y in terms of z and $\bar z$:

$$x = \tfrac12(z + \bar z)\,, \qquad y = -\tfrac{\mathrm{i}}{2}\,(z - \bar z)\,. \tag{5.58}$$

Formally, we can think of z and $\bar z$ as being independent variables. Then, using the chain rule, we shall have

$$\begin{aligned} \partial_z &\equiv \frac{\partial}{\partial z} = \frac{\partial x}{\partial z}\,\frac{\partial}{\partial x} + \frac{\partial y}{\partial z}\,\frac{\partial}{\partial y} = \tfrac12\partial_x - \tfrac{\mathrm{i}}{2}\,\partial_y\,,\\ \partial_{\bar z} &\equiv \frac{\partial}{\partial \bar z} = \frac{\partial x}{\partial \bar z}\,\frac{\partial}{\partial x} + \frac{\partial y}{\partial \bar z}\,\frac{\partial}{\partial y} = \tfrac12\partial_x + \tfrac{\mathrm{i}}{2}\,\partial_y\,, \end{aligned} \tag{5.59}$$

where $\partial_x \equiv \partial/\partial x$ and $\partial_y \equiv \partial/\partial y$. (Note that ∂_z means a partial derivative holding $\bar z$ fixed, *etc.*) So if we have a complex function $f = u + \mathrm{i}\,v$, then $\partial_{\bar z} f$ is given by

$$\partial_{\bar z} f = \tfrac12 u_x + \tfrac{\mathrm{i}}{2}\,u_y + \tfrac{\mathrm{i}}{2} v_x - \tfrac12\,v_y\,, \tag{5.60}$$

[17]A function $f(z)$ is *continuous* at z_0 if, for any given $\epsilon > 0$ (however small), we can find a number δ such that $|f(z) - f(z_0)| < \epsilon$ for all points z in D satisfying $|z - z_0| < \delta$.

which vanishes by the Cauchy-Riemann equations (5.57).[18] So the Cauchy-Riemann equations are equivalent to the statement that the function $f(z)$ depends on z but not on $\bar{z}$. We now see instantly why the function $f = |z|^2 = \bar{z}\, z$ was not in general analytic, although it was at the origin, $z = 0$.

We have seen that the real and imaginary parts u and v of an analytic function satisfy the Cauchy-Riemann equations (5.57). From these, it follows that $u_{xx} = v_{yx} = v_{xy} = -u_{yy}$, and similarly for v. In other words, u and v each satisfy Laplace's equation in two dimensions:

$$\nabla^2 u = 0\,, \qquad \nabla^2 v = 0\,, \qquad \text{where } \nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\,. \tag{5.61}$$

This is a very useful property, since it provides us with ways of solving Laplace's equation in two dimensions. It has applications in 2-dimensional electrostatics and gravity, and in hydrodynamics.

Note that another consequence of the Cauchy-Riemann equations (5.57) is that

$$u_x\, v_x + u_y\, v_y = 0\,, \tag{5.62}$$

or, in other words,

$$\vec{\nabla} u \cdot \vec{\nabla} v = 0\,, \tag{5.63}$$

where

$$\vec{\nabla} \equiv \Big(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\Big) \tag{5.64}$$

is the 2-dimensional gradient operator. Equation (5.63) says that families of curves in the (x, y) plane corresponding to $u =$ constant and $v =$ constant intersect at right-angles at all points of intersection. This is because $\vec{\nabla} u$ is perpendicular to the lines of constant u, while $\vec{\nabla} v$ is perpendicular to the lines of constant v.

5.2.1 Power Series

A very important concept in complex variable theory is the idea of a power series, and its radius of convergence. We could consider the infinite series $\sum_{n=0}^\infty a_n\, (z - z_0)^n$, but since a

[18]One might feel uneasy with treating z and $\bar{z}$ as independent variables, since one is actually the complex conjugate of the other. The proper way to show that it is a valid procedure is temporarily to introduce a genuinely independent complex variable $\tilde{z}$, and to write functions as depending on z and $\tilde{z}$, rather than z and $\bar{z}$. After performing the differentiations in this enlarged complex 2-plane, one then sets $\tilde{z} = \bar{z}$, which amounts to taking the standard "section" that defines the complex plane. It then becomes apparent that one can equally well just treat z and $\bar{z}$ as independent, and cut out the intermediate step of enlarging the dimension of the complex space.

simple shift of the origin in the complex plane allows us to take $z_0 = 0$, we may as well make life a little bit simpler by assuming this has been done. Thus, let us consider

$$f(z) = \sum_{n=0}^{\infty} a_n\, z^n\,, \tag{5.65}$$

where the a_n are constant coefficients, which may in general be complex.

A useful criterion for convergence of a series is the Cauchy test. This states that if the terms b_n in an infinite sum $\sum_n b_n$ are all non-negative, then $\sum_n b_n$ converges or diverges according to whether the limit of

$$(b_n)^{\frac{1}{n}} \tag{5.66}$$

is less than or greater than 1, as n tends to infinity.

We can apply this to determine the conditions under which the series (5.65) is *absolutely convergent*. Namely, we consider the series

$$\sum_{n=0}^{\infty} |a_n|\, |z|^n\,, \tag{5.67}$$

which is clearly a sum of non-negative terms. If

$$|a_n|^{\frac{1}{n}} \longrightarrow 1/R \tag{5.68}$$

as $n \longrightarrow \infty$, then it is evident that the power series (5.65) is absolutely convergent if $|z| < R$, and divergent if $|z| > R$. (As always, the borderline case $|z| = R$ is trickier, and depends on finer details of the coefficients a_n.) The quantity R is called the *radius of convergence* of the series. The circle of radius R (centred on the expansion point $z = 0$ in our case) is called the *circle of convergence*. The series (5.65) is absolutely convergent for any z that lies in within the circle of convergence.

We can now establish the following theorem, which is of great importance.

If $f(z)$ is defined by the power series (5.65), then $f(z)$ is an analytic function at every point within the circle of convergence.

This is all about establishing that the power series defining $f(z)$ is differentiable within the circle of convergence. Thus we define

$$\phi(z) = \sum_{(n)=1}^{\infty} n\, a_n\, z^{n-1}\,, \tag{5.69}$$

without yet prejudging that $\phi(z)$ is the derivative of $f(z)$. Suppose the series (5.65) has radius of convergence R. It follows that for any ρ such that $0 < \rho < R$, $|a_n\, \rho^n|$ must be bounded, since we know that even the entire infinite sum is bounded. We may say, then, that $|a_n\,\rho^n| < K$ for any n, where K is some positive number. Then, defining $r = |z|$, and $\eta = |h|$, it follows that if $r < \rho$ and $r + \eta < \rho$, we have

$$\frac{f(z+h) - f(z)}{h} - \phi(z) = \sum_{n=0}^{\infty} a_n \Big(\frac{(z+h)^n - z^n}{h} - n\, z^{n-1} \Big) \,. \tag{5.70}$$

Using the inequality (5.50), we have

$$\begin{aligned} \Big| \frac{(z+h)^n - z^n}{h} - n\, z^{n-1} \Big| &= \Big| \tfrac{1}{2!}\, n(n-1)\, z^{n-2}\, h + \tfrac{1}{3!}\, n(n-1)(n-2)\, z^{n-3}\, h^2 + \cdots + h^{n-1} \Big| \,, \\ &\le \tfrac{1}{2!}\, n(n-1)\, r^{n-2}\, \eta + \tfrac{1}{3!}\, n(n-1)(n-2)\, r^{n-3}\, \eta^2 + \cdots + \eta^{n-1} \,, \\ &= \frac{(r+\eta)^n - r^n}{\eta} - n\, r^{n-1} \,. \end{aligned} \tag{5.71}$$

Hence

$$\begin{aligned} \sum_{n=0}^{\infty} |a_n| \Big| \frac{(z+h)^n - z^n}{h} - n\, z^{n-1} \Big| &\le K \sum_{n=0}^{\infty} \frac{1}{\rho^n} \Big[\frac{(r+\eta)^n - r^n}{\eta} - n\, r^{n-1} \Big] \,, \\ &= K \Big[\frac{1}{\eta} \Big(\frac{\rho}{\rho - r - \eta} - \frac{\rho}{\rho - r} \Big) - \frac{\rho}{(\rho - r)^2} \Big] \,, \\ &= \frac{K\, \rho\, \eta}{(\rho - r - \eta)(\rho - r)^2} \,. \end{aligned} \tag{5.72}$$

Clearly this tends to zero as η goes to zero. This proves that $\phi(z)$ given in (5.69) is indeed the derivative of $f(z)$. Thus $f(z)$, defined by the power series (5.65), is differentiable within its circle of convergence. Since it is also manifestly single-valued, this means that it is analytic with the circle of convergence.

It is also clear that the derivative $f'(z)$, given, as we now know, by (5.69), is has the same radius of convergence as the original series for $f(z)$. This is because the limit of $|n\, a_n|^{1/n}$ as n tends to infinity is clearly the same as the limit of $|a_n|^{1/n}$. The process of differentiation can therefore be continued to higher and higher derivatives. In other words, a power series can be differentiated term by term as many times as we wish, at any point within its circle of convergence.

5.3 Contour Integration

5.3.1 Cauchy's Theorem

A very important result in the theory of complex functions is *Cauchy's Theorem*, which states:

- *If a function $f(z)$ is analytic, and it is continuous within and on a smooth closed contour C, then*

$$\oint_C f(z)\, dz = 0 \,. \tag{5.73}$$

The symbol $\oint$ denotes that the integration is taken around a closed contour; sometimes, when there is no ambiguity, we shall omit the subscript C that labels this contour.

To see what (5.73) means, consider first the following. Since $f(z) = u(x,y) + \mathrm{i}\, v(x,y)$, and $z = x + \mathrm{i}\, y$, we may write (5.73) as

$$\oint_C f(z)\, dz = \oint_C (u\, dx - v\, dy) + \mathrm{i} \oint_C (v\, dx + u\, dy)\,, \tag{5.74}$$

where we have separated the original integral into its real and imaginary parts. Written in this way, each of the contour integrals can be seen to be nothing but a closed line integral of the kind familiar, for example, in electromagnetism. The only difference here is that we are in two dimensions rather than three. However, we still have the concept Stokes' Theorem, known as *Green's Theorem* in two dimensions, which asserts that

$$\oint \vec{E} \cdot d\vec{\ell} = \int_S \vec{\nabla} \times \vec{E} \cdot d\vec{S}\,, \tag{5.75}$$

where C is a closed curve bounding a domain S, and $\vec{E}$ is any vector field defined in S and on C, with well-defined derivatives in S. In two dimensions, the curl operator $\vec{\nabla}\times$ just means

$$\vec{\nabla} \times \vec{E} = \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}\,. \tag{5.76}$$

(It is effectively like the z component of the three-dimensional curl.) $\vec{E} \cdot d\vec{\ell}$ means $E_x\, dx + E_y\, dy$, and the area element $d\vec{S}$ will just be $dx\, dy$.

Applying Green's theorem to the integrals in (5.74), we therefore obtain

$$\oint_C f(z)\, dz = -\int_S \Big(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\Big)\, dx\, dy + \mathrm{i} \int_S \Big(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\Big)\, dx\, dy\,. \tag{5.77}$$

But the integrands here are precisely the quantities that vanish by virtue of the Cauchy-Riemann equations (5.57), and thus we see that $\oint f(z)\, dz = 0$, verifying Cauchy's theorem.

An alternative proof of Cauchy's theorem can be given as follows. Define first the slightly more general integral

$$F(\lambda) \equiv \lambda \oint f(\lambda z)\, dz\,; \qquad 0 \le \lambda \le 1\,, \tag{5.78}$$

where λ is a constant parameter that can be freely chosen in the interval $0 \le \lambda \le 1$. Cauchy's theorem is therefore the statement that $F(1) = 0$. To show this, first differentiate $F(\lambda)$ with respect to λ:

$$F'(\lambda) = \oint f(\lambda z)\, dz + \lambda \oint z\, f'(\lambda z)\, dz\,. \tag{5.79}$$

(The prime symbol $'$ always means the derivative of a function with respect to its argument.) Now integrate the second term by parts, giving

$$\begin{aligned} F'(\lambda) &= \oint f(\lambda z)\, dz + \lambda\Big([\lambda^{-1}\, z\, f(\lambda z)] - \lambda^{-1} \oint f(\lambda z)\, dz\Big) \\ &= [\lambda^{-1}\, z\, f(\lambda z)]\,, \end{aligned} \tag{5.80}$$

where the square brackets indicate that we take the difference between the values of the enclosed quantity at the beginning and end of the integration range. But since we are integrating around a closed curve, and since $z\, f(\lambda z)$ is a single-valued function, this must vanish. Thus we have established that $F'(\lambda) = 0$, implying that $F(\lambda) =$ constant. We can determine this constant by considering any value of λ we wish. Taking $\lambda = 0$, it is clear from (5.78) that $F(0) = 0$, whence $F(1) = 0$, proving Cauchy's theorem.

Why did we appear not to need the Cauchy-Riemann equations (5.57) in this proof? The answer, of course, is that effectively we did, since we assumed that we could sensibly talk about the derivative of f, called f'. As we saw when we discussed the Cauchy-Riemann equations, they are the consequence of requiring that $f'(z)$ have a well-defined meaning.

Cauchy's theorem has very important implications in the theory of integration of complex functions. One of these is that if $f(z)$ is an analytic function in some domain D, then if we integrate $f(z)$ from points z_1 to z_2 within D the answer

$$\int_{z_1}^{z_2} f(z)\, dz \tag{5.81}$$

is independent of the path of integration within D. This follows immediately by noting that if we consider two integration paths P_1 and P_2 then the total path consisting of integration from z_1 to z_2 along P_1, and then back to z_1 in the negative direction along P_2 constitutes a closed curve $C = P_1 - P_2$ within D. Thus Cauchy's theorem tells us that

$$0 = \oint_C f(z)\, dz = \int_{P_1} f(z)\, dz - \int_{P_2} f(z)\, dz\,. \tag{5.82}$$

Another related implication from Cauchy's theorem is that it is possible to define an *indefinite integral* of $f(z)$, by

$$g(z) = \int_{z_0}^{z} f(z')\, dz'\,, \tag{5.83}$$

where the contour of integration can be taken to be any path within the domain of analyticity. Notice that the integrated function, $g(z)$, has the same domain of analyticity as the integrand $f(z)$. To show this, we just have to show that the derivative of $g(z)$ is unique. This (almost self-evident) property can be made evident by considering

$$\frac{g(z) - g(\zeta)}{z - \zeta} - f(\zeta) = \frac{\int_\zeta^z (f(z') - f(\zeta))\, dz'}{z - \zeta}\,. \tag{5.84}$$

Since $f(z)$ is continuous and single-valued, it follows that $|f(z') - f(\zeta)|$ will tend to zero at least as fast as $|z - \zeta|$ for any point z' on a direct path joining ζ to z, as z approaches ζ. Together with the fact that the integration range itself is tending to zero in this limit, it is evident that the right-hand side in (5.84) will tend to zero as ζ approaches ζ, implying therefore that $g'(z)$ exists and is equal to $f(z)$.

A third very important implication from Cauchy's theorem is that *if a function $f(z)$ that* does *contain some sort of singularities within a closed curve C is integrated around C, then the result will be unchanged if the contour is deformed in any way, provided that it does not cross any singularity of $f(z)$ during the deformation.* This property will prove to be invaluable later, when we want to perform explicit evaluations of contour integrals.

Finally, on the subject of Cauchy's theorem, let us note that we can turn it around, and effectively use it as a *definition* of an analytic function. This is the content of *Morera's Theorem*, which states:

- *If $f(z)$ is continuous and single-valued within a closed contour C, and if $\oint f(z)\, dz = 0$ for any closed contour within C, then $f(z)$ is analytic within C.*

This can provide a useful way of testing whether a function is analytic in some domain.

5.3.2 Cauchy's Integral Formula

Suppose that the function $f(z)$ is analytic in a domain D. Consider the integral

$$G(a) = \oint_C \frac{f(z)}{z-a}\, dz\,, \tag{5.85}$$

where the contour C is any closed curve within D. There are three cases to consider, depending on whether the point a lies inside, on, or outside the contour of integration C.

Consider first the case when a lies within C. By an observation in the previous section, we know that the value of the integral (5.85) will not alter if we deform the contour in any way provided that the deformation does not cross over the point $z = a$. We can exploit this in order to make life simple, by deforming the contour into a small circle C', of radius ϵ, centred on the point a. Thus we may write

$$z - a = \epsilon\, e^{\mathrm{i}\theta}\,, \tag{5.86}$$

with the deformed contour C' being parameterised by taking θ from 0 to 2π.[19]

[19]Note that this means that we define a *positively-oriented* contour to be one whose path runs *anti-clockwise*, in the direction of *increasing* θ. Expressed in a coordinate-invariant way, a positively-oriented closed contour is one for which the interior lies to the *left* as you walk along the path.

Thus we have $dz = \mathrm{i}\,\epsilon\, e^{\mathrm{i}\theta}\, d\theta$, and so

$$G(a) = \mathrm{i} \int_0^{2\pi} f(a + \epsilon\, e^{\mathrm{i}\theta})\, d\theta = \mathrm{i}\, f(a) \int_0^{2\pi} d\theta + \mathrm{i} \int_0^{2\pi} [f(a + \epsilon\, e^{\mathrm{i}\theta}) - f(a)]\, d\theta\,. \tag{5.87}$$

In the limit as ϵ tends to zero, the continuity of the function $f(z)$ implies that the last integral will vanish, since $f(a + \epsilon\, e^{\mathrm{i}\,\theta}) = f(a) + f'(a)\, \epsilon\, e^{\mathrm{i}\,\theta} + \cdots$, and so we have that if $f(z)$ is analytic within and on any closed contour C then

$$\oint_C \frac{f(z)}{z-a}\, dz = 2\pi\, \mathrm{i}\, f(a)\,, \tag{5.88}$$

provided that C contains the point $z = a$. This is *Cauchy's integral formula.*

Obviously if the point $z = a$ were to lie outside the contour C, then we would, by Cauchy's theorem, have

$$\oint_C \frac{f(z)}{z-a}\, dz = 0\,, \tag{5.89}$$

since then the integrand would be a function that was analytic within C.

The third case to consider is when the point a lies exactly on the path of the contour C. It is somewhat a matter of definition, as to how we should handle this case. The most reasonable thing is to decide, like in the Judgement of Solomon, that the point is to be viewed as being split into two, with half of it lying inside the contour, and half outside. Thus if a lies on C we shall have

$$\oint_C \frac{f(z)}{z-a}\, dz = \pi\, \mathrm{i}\, f(a)\,. \tag{5.90}$$

We can view the Cauchy integral formula as a way of evaluating an analytic function at a point z in terms of a contour integral around any closed curve C that contains z:

$$f(z) = \frac{1}{2\pi\, \mathrm{i}} \oint_C \frac{f(\zeta)\, d\zeta}{\zeta - z}\,. \tag{5.91}$$

A very useful consequence from this is that we can use it also to express the derivatives of $f(z)$ in terms of contour integrals. Essentially, one just differentiates (5.91) with respect to z, meaning that on the right-hand side it is only the function $(\zeta - z)^{-1}$ that is differentiated. We ought to be a little careful just once to verify that this "differentiation under the integral" is justified, so that having established the validity, we can be cavalier about it in the future. The demonstration is in any case pretty simple. We have

$$\begin{aligned} \frac{f(z+h) - f(z)}{h} &= \frac{1}{2\pi\, \mathrm{i}} \oint \frac{f(\zeta)}{h} \Big(\frac{1}{\zeta - z - h} - \frac{1}{\zeta - z} \Big)\, d\zeta\,, \\ &= \frac{1}{2\pi\, \mathrm{i}} \oint \frac{f(\zeta)\, d\zeta}{(\zeta - z)(\zeta - z - h)}\,. \end{aligned} \tag{5.92}$$

Now in the limit when $h \longrightarrow 0$ the left-hand side becomes $f'(z)$, and thus we get

$$f'(z) = \frac{1}{2\pi\,\mathrm{i}} \oint \frac{f(\zeta)\,d\zeta}{(\zeta - z)^2}\,. \tag{5.93}$$

The question of the validity of this process, in which we have taken the limit $h \longrightarrow 0$ under the integration, comes down to whether it was valid to assume that

$$\begin{aligned} T &\equiv -\oint f(\zeta)\Big(\frac{1}{(\zeta-z)^2} - \frac{1}{(\zeta - z - h)(\zeta - z)}\Big)\,d\zeta \\ &= h \oint \frac{f(\zeta)\,d\zeta}{(\zeta - z)^2\,(\zeta - z - h)} \end{aligned} \tag{5.94}$$

vanishes as h tends to zero. Now it is evident that

$$|T| \le \frac{|h|\,M\,L}{b^2\,(b - |h|)}\,, \tag{5.95}$$

where M is the maximum value of $|f(\zeta)|$ on the contour, L is the length of the contour, and b is the minimum value of of $|\zeta - z|$ on the contour. These are all fixed numbers, independent of h, and so we see that indeed T must vanish as h is taken to zero.

More generally, by continuing the above procedure, we can show that the n'th derivative of $f(z)$ is given by

$$f^{(n)}(z) = \frac{1}{2\pi\,\mathrm{i}} \oint f(\zeta)\,\frac{d^n}{dz^n}\Big(\frac{1}{\zeta - z}\Big)\,d\zeta\,, \tag{5.96}$$

or, in other words,

$$f^{(n)}(z) = \frac{n!}{2\pi\,\mathrm{i}} \oint_C \frac{f(\zeta)\,d\zeta}{(\zeta - z)^{n+1}}\,. \tag{5.97}$$

Note that since all the derivatives of $f(z)$ exist, for all point C within the contour C, it follows that $f^{(n)}(z)$ is analytic within C for any n.

5.3.3 The Taylor Series

We can use Cauchy's integral formula to derive Taylor's theorem for the expansion of a function $f(z)$ around a point $z = a$ at which $f(z)$ is analytic. An important outcome from this will be that we shall see that the radius of convergence of the Taylor series extends up to the singularity of $f(z)$ that is nearest to $z = a$.

From Cauchy's integral formula we have that if $f(z)$ is analytic inside and on a contour C, and if $z = a + h$ lies inside C, then

$$f(a + h) = \frac{1}{2\pi\,\mathrm{i}} \oint \frac{f(\zeta)\,d\zeta}{\zeta - a - h}\,. \tag{5.98}$$

Now, bearing in mind that the geometric series $\sum_{n=0}^N x^n$ sums to give $(1 - x^{N+1})\,(1-x)^{-1}$, we have that

$$\sum_{n=0}^N \frac{h^n}{(\zeta - a)^{n+1}} = \frac{1}{\zeta - a - h} - \frac{h^{N+1}}{(\zeta - a - h)\,(\zeta - a)^{N+1}}\,. \tag{5.99}$$

We can use this identity as an expression for $\frac{1}{z-a-h}$ in (5.98), implying that

$$f(a+h) = \sum_{n=0}^{N} \frac{h^n}{2\pi\,\mathrm{i}} \oint \frac{f(\zeta)\,d\zeta}{(\zeta-a)^{n+1}} + \frac{h^{N+1}}{2\pi\,\mathrm{i}} \oint \frac{f(\zeta)\,d\zeta}{(\zeta-a-h)\,(\zeta-a)^{N+1}}\,. \tag{5.100}$$

In other words, in view of our previous result (5.97), we have

$$f(a+h) = \sum_{n=0}^{N} \frac{h^n}{n!}\, f^{(n)}(a) + R_N\,, \tag{5.101}$$

where the "remainder" term R_N is given by

$$R_N = \frac{h^{N+1}}{2\pi\,\mathrm{i}} \oint_C \frac{f(\zeta)\,d\zeta}{(\zeta-a-h)\,(\zeta-a)^{N+1}}\,. \tag{5.102}$$

Now, if M denotes the maximum value of $|f(\zeta)|$ on the contour C, then by taking C to be a circle of radius r centred on $\zeta = a$, we shall have

$$|R_N| \le \frac{|h|^{N+1}\, M\, r}{(r-|h|)\, r^{N+1}} = \frac{M\, r}{r-|h|} \Big(\frac{|h|}{r}\Big)^{N+1}\,. \tag{5.103}$$

Thus if we choose h such that $|h| < r$, it follows that as N is sent to infinity, R_N will go to zero. This means that the Taylor series

$$f(a+h) = \sum_{n=0}^{\infty} \frac{h^n}{n!}\, f^{(n)}(a)\,, \tag{5.104}$$

or in other words,

$$f(z) = \sum_{n=0}^{\infty} \frac{(z-a)^n}{n!}\, f^{(n)}(a)\,, \tag{5.105}$$

will be convergent for any z lying within the circle of radius r centred on $z = a$. But we can choose this circle to be as large as we like, provided that it does not enclose any singularity of $f(z)$. Therefore, it follows that the radius of convergence of the Taylor series (5.104) is precisely equal to the distance between $z = a$ and the nearest singularity of $f(z)$.

5.3.4 The Laurent Series

Suppose now that we want to expand $f(z)$ around a point $z = a$ where $f(z)$ has a singularity. Clearly the previous Taylor expansion will no longer work. However, depending upon the nature of the singularity at $z = a$, we may be able to construct a more general kind of series expansion, known as a Laurent series. To do this, consider two concentric circles C_1 and C_2, centred on the point $z = a$, where C_1 has a larger radius that takes it out as far as possible before hitting the next singularity of $f(z)$, while C_2 is an arbitrarily small circle enclosing a. Take the path C_1 to be anticlockwise, while the path C_2 is clockwise. We can

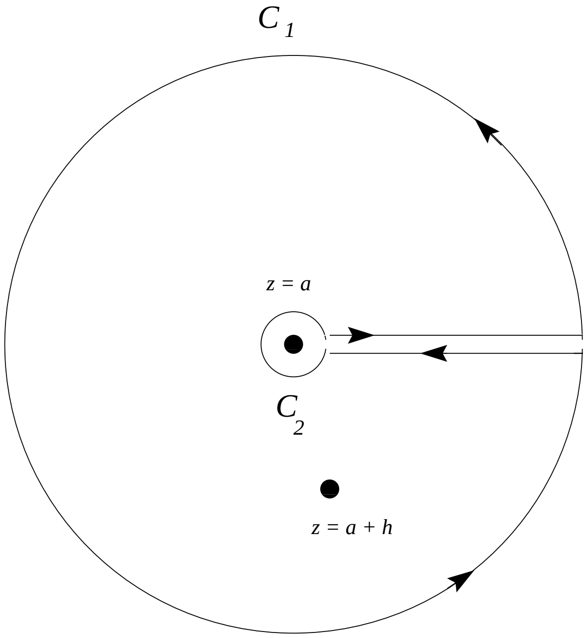

Figure 1: The contour $C = C_1 + C_2$ for Cauchy's integral

make C_1 and C_2 into a single closed contour C, by joining them along a narrow "causeway," as shown in Figure 1.

The idea is that we will take a limit where the width of the "causeway" joining the innner and outer circles shrinks to zero. In the region of the complex plane under discussion, the function $f(z)$ has, by assumption, only an isolated singularity at $z = a$.

Now consider Cauchy's integral formula for this contour, which will give

$$f(a+h) = \frac{1}{2\pi\,\mathrm{i}} \oint_C \frac{f(\zeta)\,d\zeta}{\zeta - a - h}\,. \tag{5.106}$$

The reason for this is that the closed contour C encloses no singularities except for the pole at $\zeta = a + h$. In particular, it avoids the singularity of $f(z)$ at $z = a$. Since the integrand is non-singular in the neighbourhood of the "causeway," we see that when the width of the causeway is taken to zero, we shall find that the integration along the lower "road" heading in from C_1 to C_2 will be exactly cancelled by the integration in the opposite direction along the upper "road" heading out from C_2 to C_1. In this sense, therefore, we can disregard the contribution of the causeway, and just make the replacement that

$$\oint_C \longrightarrow \oint_{C_1} + \oint_{C_2}\,. \tag{5.107}$$

We can therefore write (5.106) as

$$f(a+h) = \frac{1}{2\pi\,\mathrm{i}} \oint_{C_1} \frac{f(\zeta)\,d\zeta}{\zeta - a - h} + \frac{1}{2\pi\,\mathrm{i}} \oint_{C_2} \frac{f(\zeta)\,d\zeta}{\zeta - a - h}\,. \tag{5.108}$$

For the first integral, around the large circle C_1, we can use the same expansion for $(\zeta - a - h)^{-1}$ as we used in the Taylor series previously, obtained by setting $N = \infty$ in (5.99), and using the fact that the second term on the right-hand side then vanishes, since $h^{N+1}/|\zeta - a|^{N+1}$ goes to zero on C_1 when N goes to infinity, as a result of the radius of C_1 being larger than $|h|$. In other words, we expand $(\zeta - a - h)^{-1}$ as

$$
\begin{aligned}
\frac{1}{\zeta - a - h} &= \frac{1}{(\zeta - a)(1 - h\,(\zeta - a)^{-1})}\,, \\
&= \frac{1}{\zeta - a}\Big(1 + \frac{h}{\zeta - a} + \frac{h^2}{(\zeta - a)^2} + \cdots\Big)\,, \\
&= \sum_{n=0}^{\infty} \frac{h^n}{(\zeta - a)^{n+1}}\,.
\end{aligned}
\tag{5.109}
$$

On the other hand, in the second integral in (5.108) we can expand $(\zeta - a - h)^{-1}$ in a series valid for $|\zeta - a| << |h|$, namely

$$
\begin{aligned}
\frac{1}{\zeta - a - h} &= -\frac{1}{h(1 - (\zeta - a)\,h^{-1})}\,, \\
&= -\frac{1}{h}\Big(1 + \frac{\zeta - a}{h} + \frac{(\zeta - a)^2}{h^2} + \cdots\Big)\,, \\
&= -\sum_{n=1}^{\infty} \frac{(\zeta - a)^{n-1}}{h^n}\,.
\end{aligned}
\tag{5.110}
$$

Thus we find

$$
f(a + h) = \frac{1}{2\pi\,\mathrm{i}} \sum_{n=0}^{\infty} h^n \oint_{C_1} \frac{f(\zeta)\,d\zeta}{(\zeta - a)^{n+1}} + \frac{1}{2\pi\,\mathrm{i}} \sum_{n=1}^{\infty} \frac{1}{h^n} \oint_{C_2^+} f(\zeta)\,(\zeta - a)^{n-1}\,d\zeta\,, \tag{5.111}
$$

where we define C_2^+ to mean the contour C_2 but with the direction of the integration path reversed, i.e. C_2^+ runs *anti-clockwise* around the point $\zeta = a$, which means it is now the standard *positive* direction for a contour. Thus we have

$$
f(a + h) = \sum_{n=-\infty}^{\infty} a_n\,h^n\,, \tag{5.112}
$$

where the coefficients a_n are given by

$$
a_n = \frac{1}{2\pi\,\mathrm{i}} \oint \frac{f(\zeta)\,d\zeta}{(\zeta - a)^{n+1}}\,. \tag{5.113}
$$

Here, the integration contour is C_1 when evaluating a_n for $n \ge 0$, and C_2^+ when evaluating a_n for $n < 0$. Notice that we can in fact just as well choose to use the contour C_1 for the $n < 0$ integrals too, since the deformation of the contour C_2^+ into C_1 does not cross any singularities of the integrand when $n < 0$.

Note that using the original variable $z = a + h$, (5.112) is written as

$$f(z) = \sum_{n=-\infty}^{\infty} a_n\,(z-a)^n\,. \tag{5.114}$$

The expansion in (5.114) is known as the *Laurent Series*. By similar arguments to those we used for the Taylor series, one can see that the series converges in an annulus whose larger radius is defined by the contour C_1. This contour could be chosen to be the largest possible circle centred on the singularity of $f(z)$ at $z = a$ that does not enclose any other singularity of $f(z)$.

In the Laurent series, the function $f(z)$ has been split as the sum of two parts:

$$\begin{aligned} f(z) &= f_+(z) + f_-(z)\,, & (5.115)\\ f_+(z) &\equiv \sum_{n\ge 0} a_n\,(z-a)^n\,, \qquad f_-(z) \equiv \sum_{m\ge 1} \frac{a_{-m}}{(z-a)^m}\,. & (5.116)\end{aligned}$$

The part $f_+(z)$ (the terms with $n \ge 0$ in (5.114)) is analytic everywhere inside the larger circle C_1. The part $f_-(z)$ (the terms with $n \le -1$ in (5.114)) is analytic everywhere outside the small circle C_2 enclosing the singularity as $z = a$.

In practice, one commonly wants to work out just the first few terms in the Laurent expansion of a function around a singular point. For example, it is often of interest to know the singular terms, corresponding to the inverse powers of $(z - a)$ in (5.114). If the function in question has a pole of degree N at the expansion point, then there will just be N singular terms, corresponding to the powers $(z - a)^{-N}$ down to $(z - a)^{-1}$. For reasons that we shall see later, the coefficient of $(z - a)^{-1}$ is often of particular interest.

Determining the first few terms in the expansion of a function with a pole at $z = a$ is usually pretty simple, and can just be done by elementary methods. Suppose, for example, we have the function

$$f(z) = \frac{g(z)}{z^N}\,, \tag{5.117}$$

where $g(z)$ is analytic, and that we want to find the Laurent expansion around the point $z = 0$. Since $g(z)$ is analytic, it has a Taylor expansion, which we can write as

$$g(z) = \sum_{m\ge 0} b_m\, z^m\,. \tag{5.118}$$

The Laurent expansion for $f(z)$ is therefore

$$\begin{aligned} f(z) &= \frac{1}{z^N} \sum_{m\ge 0} b_m\, z^m \\ &= \sum_{m\ge 0} b_m\, z^{m-N} \end{aligned}$$

$$= \sum_{n\ge -N} b_{n+N}\, z^n\,. \qquad (5.119)$$

For example, the Laurent expansion of $f(z) = z^{-2}\, e^z$ is given by

$$\begin{aligned} f(z) &= \frac{1}{z^2}\,\Big(1 + z + \tfrac12 z^2 + \tfrac16 z^3 + \cdots\Big) \\ &= \frac{1}{z^2} + \frac{1}{z} + \tfrac12 + \tfrac16 z + \cdots\,. \end{aligned} \qquad (5.120)$$

In more complicated examples, there might be an analytic function that goes to zero in the denominator of the function $f(z)$. We can still work out the first few terms in the Laurent expansion by elementary methods, by writing out the Taylor expansion of the function in the denominator. Consider, for example, the function $f(z) = 1/\sin z$, to be expanding in a Laurent series around $z = 0$. We just write out the first few terms in the Taylor series for $\sin z$,

$$\begin{aligned} \sin z &= z - \tfrac16 z^3 + \tfrac{1}{120} z^5 + \cdots \\ &= z\,\Big(1 - \tfrac16 z^2 + \tfrac{1}{120} z^4 + \cdots\Big)\,. \end{aligned} \qquad (5.121)$$

Notice that on the second line, we have pulled out the overall factor of z, so that what remains inside the parentheses is an analytic function that does not go to zero at $z = 0$. Now, we write

$$f(z) = \frac{1}{\sin z} = \frac{1}{z}\,\Big(1 - \tfrac16 z^2 + \tfrac{1}{120} z^4 + \cdots\Big)^{-1}\,, \qquad (5.122)$$

and the problem has reduced to the kind we discussed previously. Making the expansion of the term in parentheses using $(1+x)^{-1} = 1 - x + x^2 - x^3 + \cdots$, we get

$$f(z) = \frac{1}{z}\,\Big(1 + \tfrac16 z^2 + \tfrac{7}{360} z^4 + \cdots\Big)\,, \qquad (5.123)$$

and hence the Laurent expansion is

$$\frac{1}{\sin z} = \frac{1}{z} + \tfrac16 z + \tfrac{7}{360} z^3 + \cdots\,. \qquad (5.124)$$

Note that if we had only wanted to know the pole term, we would not have needed to push the series expansion as far as we just did. So as a practical tip, time can be saved by working just to the order needed, and no more, when performing the expansion. (One must take care, though, to be sure to take the expansion far enough.)

5.4 Classification of Singularities

We are now in a position to classify the types of singularity that a function of a complex variable may possess.

Suppose that $f(z)$ has a singularity at $z = a$, and that its Laurent expansion for $f(a+h)$, given in general in (5.112), actually terminates at some specific negative value of n, say $n = -N$. Thus we have

$$f(a+h) = \sum_{n=-N}^{\infty} a_n\, h^n\,. \tag{5.125}$$

We then say that $f(z)$ has a *pole* of order N at $z = a$. In other words, as z approaches a the function $f(z)$ has the behaviour

$$f(z) = \frac{a_{-N}}{(z-a)^N} + \text{ less singular terms}\,. \tag{5.126}$$

If, on the other hand, the sum over negative values of n in (5.112) does not terminate, but goes on to $n = -\infty$, then the function $f(z)$ has an *essential singularity* at $z = a$. A classic example is the function

$$f(z) = e^{\frac{1}{z}}\,. \tag{5.127}$$

This has the Laurent expansion

$$f(z) = \sum_{n=0}^{\infty} \frac{1}{n!\, z^n} \tag{5.128}$$

around $z = 0$, which is obtained simply by taking the usual Taylor expansion of

$$e^w = \sum_{n\ge 0} \frac{w^n}{n!} \tag{5.129}$$

and setting $w = 1/z$. The Laurent series (5.128) has terms in arbitrarily negative powers of z, and so $z = 0$ is an essential singularity.

Functions have quite a complicated behaviour near an essential singularity. For example, if z approaches zero along the positive real axis, $e^{1/z}$ tends to infinity. On the other hand, if the approach to zero is along the negative real axis, $e^{1/z}$ instead tends to zero. An approach to $z = 0$ along the imaginary axis causes $e^{1/z}$ to have unit modulus, but with an ever-increasing phase rotation. In fact a function $f(z)$ with an essential singularity can take on any value, for z near to the singular point.

Note that the Laurent expansion (5.112) that we have been discussing here is applicable only if the singularity of $f(z)$ is an *isolated* one.[20] There can also exist singularities of a different kind, which are neither poles nor essential singularities. Consider, for example, the functions $f(z) = \sqrt{z}$, or $f(z) = \log z$. Neither of these can be expanded in a Laurent series around $z = 0$. They are both discontinuous along an entire semi-infinite line starting

[20]By definition, if a function $f(z)$ has a singularity at $z = a$, then it is an isolated singularity if $f(z)$ can be expanded in a Laurent series around $z = a$.

from the point $z = 0$. Thus the singularity at $z = 0$ is not an isolated one; it is called a *branch point.* We shall discuss these in more detail later.

For now, just take note of the fact that a singularity in a function does not necessarily mean that the function is infinite there. *By definition, a function $f(z)$ is singular at $z = a$ if it is not analytic at $z = a$.* Thus, for example, $f(z) = z^{1/2}$ is singular at $z = 0$, even though $f(0) = 0$. This can be seen from the fact that we cannot expand $z^{1/2}$ as a power series around $z = 0$, and therefore $z^{1/2}$ cannot be analytic there.

For now, let us look in a bit more detail at functions with isolated singularities.

5.4.1 Entire Functions

A very important, and initially perhaps rather surprising, result is the following, known as *Liouville's Theorem*:

> *A function $f(z)$ that is analytic for all finite values of z and is bounded everywhere is a constant.*

Note that when we say $f(z)$ is bounded everywhere (at finite z), we mean that there exists some positive number S, which is independent of z, such that

$$|f(z)| \le S \tag{5.130}$$

for all finite z.

We can prove Liouville's theorem using the result obtained earlier from Cauchy's integral formula, for $f'(a)$:

$$f'(a) = \frac{1}{2\pi\,\mathrm{i}} \oint \frac{f(z)\,dz}{(z-a)^2}\,. \tag{5.131}$$

Take the contour of integration to be a circle of radius R centred on $z = a$. Since we are assuming that $f(z)$ is bounded, we may take $|f(z)| \le M$ for all points z on the contour, where M is some finite positive number. Then, using (5.131), we must have

$$|f'(a)| \le \Big(\frac{M}{2\pi\,R^2}\Big)\,(2\pi\,R) = \frac{M}{R}\,. \tag{5.132}$$

Thus by taking R to infinity, and recalling our assumption that $f(z)$ remains bounded for all finite z (meaning that M is finite, in fact $M \le S$, no matter how large R is), we see that $f'(a)$ must be zero. Thus $f(a)$ is a constant, independent of a. Thus Liouville's theorem is established.

An illustration of Liouville's theorem can be given with the following example. Suppose we try to construct an analytic function that is well-behaved, and bounded, everywhere. If we were considering real functions as opposed to complex analytic functions, we might consider a function such as

$$f(x) = \frac{1}{1+x^2}\,, \tag{5.133}$$

which rather boringly falls off to zero as x tends to $+\infty$ or $-\infty$, having attained the exciting peak of $f = 1$ at the origin. Thus as a real function of x, we have $|f(x)| \le 1$ everywhere. However, viewed as a function of the variable z in the complex plane, it is unbounded:

$$f(z) = \frac{1}{1+z^2} = \frac{1}{(z-\mathrm{i})(z+\mathrm{i})} = \frac{\mathrm{i}}{2(z+\mathrm{i})} - \frac{\mathrm{i}}{2(z-\mathrm{i})},. \tag{5.134}$$

Thus the function $f(z)$ actually has poles at $z = \pm\mathrm{i}$, away from the z axis. Of course we could consider instead the function

$$g(z) = \frac{1}{1+|z|^2}\,, \tag{5.135}$$

which certainly satisfies $|g(z)| \le 1$ everywhere. But $g(z)$ is not analytic (since it depends on $\bar z$ as well as z.)

Liouville's theorem tells us that any bounded analytic function we try to construct is inevitably going to have singularities somewhere, unless we are content with the humble constant function.

A similar argument to the above allows us to extend Liouville's theorem to the following:

If $f(z)$ is analytic for all finite z, and if $|f(z)|$ is bounded by $S\,|z|^k$ for some integer k and some constant S as z approaches infinity, then $f(z)$ is a polynomial of degree $\le k$.

To show this, we follow the same strategy as before, by using the higher-derivative consequences of Cauchy's integral:

$$f^{(n)}(a) = \frac{n!}{2\pi\,\mathrm{i}} \oint \frac{f(z)\,dz}{(z-a)^{n+1}}\,. \tag{5.136}$$

Assume that $|f(z)| \le M\,|z|^k$ on the contour at radius R centred on $z = a$. Then we have

$$|f^{(n)}(a)| \le \Big(\frac{n!\,M\,R^k}{2\pi\,R^{n+1}}\Big)\,(2\pi\,R) = n!\,M\,R^{k-n}\,. \tag{5.137}$$

Thus we see that as R tends to infinity, all the terms with $k < n$ will vanish (since we shall always have $M \le S$, where S is some fixed number), and so

$$f^{(n)}(a) = 0\,, \qquad \text{for}\ \ n > k\,. \tag{5.138}$$

But this is just telling us that $f(z)$ is a polynomial in z with z^k as its highest power, which proves the theorem. Liouville's theorem itself is just the special case $k = 0$.

A function $f(z)$ that is a polynomial in z of degree k,

$$f(z) = \sum_{n=0}^{k} a_n\, z^n \,, \tag{5.139}$$

is clearly analytic for all finite values of z. However, if $k > 0$ it will inevitably have a pole at infinity. To see this, we use the usual trick of making the coordinate transformation

$$\zeta = \frac{1}{z} \,, \tag{5.140}$$

and then looking at the behaviour of the function $f(1/\zeta)$ at $\zeta = 0$. Clearly, for a polynomial of degree k of the form (5.139), we shall get

$$f(1/\zeta) = \sum_{n=0}^{k} a_n\, \zeta^{-n} \,, \tag{5.141}$$

implying that there are poles of orders up to and including k at $z = \infty$.

Complex functions that are analytic in every finite region in the complex plane are called *entire functions*. All polynomials, as we have seen, are therefore entire functions. Another example is the exponential function e^z, defined by the power-series expansion

$$e^z = \sum_{n=0}^{\infty} \frac{z^n}{n!} \,. \tag{5.142}$$

By the Cauchy test for the convergence of series, we see that $(|z|^n/n!)^{1/n}$ tends to zero as n tends to infinity, for any finite $|z|$, and so the exponential is analytic for all finite z. Of course the situation at infinity is another story; here, one has to look at $e^{1/\zeta}$ as ζ tends to zero, and as we saw previously this has an essential singularity, which is more divergent than any finite-order pole. Other examples of entire functions are $\cos z$, and the Bessel function of integer order, $J_n(z)$. The Bessel function has the power-series expansion

$$J_n(z) = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{\ell!\,(n+\ell)!} \Big(\frac{z}{2}\Big)^{n+2\ell} \,. \tag{5.143}$$

Of course we know from Liouville's theorem that any interesting entire function (i.e. anything except the purely constant function) must have some sort of singularity at infinity.

5.4.2 Meromorphic Functions

Entire functions are analytic everywhere except at infinity. Next on the list are *meromorphic functions*:

A Meromorphic Function $f(z)$ is analytic everywhere in the complex plane (including infinity), except for isolated poles.

We insist, in the definition of a meromorphic function, that the only singularities that are allowed are *poles*, and not, for example, *essential singularities.* Note that we also insist, in this definition of a strictly meromorphic function, that it either be analytic also at infinity, or at worst, have a pole at infinity.

The number of poles in a meromorphic function must be finite. This follows from the fact that if there were an infinite number then there would exist some singular point, either at finite z or at $z = \infty$, which would not be isolated, thus contradicting the definition of an everywhere-meromorphic function. For example; suppose we had a function with poles at all the integers along the real axis. These would appear to be isolated, since each one is unit distance from the next. However, these poles actually have an accumulation point at infinity, as can be seen by writing $z = 1/\zeta$ and looking near $\zeta = 0$. Thus a function of this type will actually have a bad singularity at infinity, We shall in fact be studying such an example later.

Any meromorphic function $f(z)$ can be written as a ratio of two polynomials. Such a ratio is known as a *rational function.* To see why we can always write $f(z)$ in this way, we have only to make use of the observation above that the number of poles must be finite. Let the number of poles at finite z be N. Thus at a set of N points z_n in the complex plane, the function $f(z)$ has poles of orders d_n. It follows that the function

$$g(z) \equiv f(z) \prod_{n=1}^{N} (z - z_n)^{d_n} \tag{5.144}$$

must be analytic everywhere (except possibly at infinity), since we have cleverly arranged to cancel out every pole at finite z. Even if $f(z)$ does have a pole at infinity, it follows from (5.144) that $g(z)$ will diverge no faster than $|z|^k$ for some finite integer k. But we saw earlier, in the generalisation of Liouville's theorem, that any such function must be a polynomial of degree $\le k$. Thus we conclude that $f(z)$ is a ratio of polynomials:

$$f(z) = \frac{g(z)}{\prod_{n=1}^{N} (z - z_n)^{d_n}} \,. \tag{5.145}$$

The fact that a meromorphic function can be expressed as a ratio of polynomials can be extremely useful.

A ratio of two polynomials can be expanded out as a sum of partial fractions. For example

$$\frac{1+z^2}{1-z^2} = \frac{1}{z+1} - \frac{1}{z-1} - 1\,. \tag{5.146}$$

Therefore it follows that a function $f(z)$ that is meromorphic can be expanded out as a sum of partial fractions in that region. For a strictly meromorphic function, this sum will be a finite one (since there are only finitely many poles, each of finite order).

Having introduced the notion of a strictly meromorphic function, it is also useful to introduce a slightly less strict notion of meromorphicity. Thus, we can define the notion of a function that is meromorphic *within a restricted region.* Thus a function is said to be meromorphic in a domain D in the complex plane if it is analytic except for pole singularities in the domain D. The previous definition of a meromorphic function thus corresponds to the case where D is the entire complex plane, *including infinity.* A very common situation for a more restricted meromorphic function is when we consider functions that are *meromorphic in the finite complex plane.* Such functions are analytic except for isolated pole singularities everywhere in the finite complex plane, but they are allowed to have "worse" singularities (such as essential singularities) at infinity. Notice in particular that such a function *is* now allowed to have an infinite number of isolated poles in the finite complex plane (since we are now allowing there to be an accumulation point at infinity).

Let us consider an example of a function $f(z)$ that is meromorphic in some region, and furthermore where every pole is of order 1. This is in fact a very common circumstance. As a piece of terminology, a pole of order 1 is also known as a *simple pole.* Let us assume that the poles are located at the points a_n, numbered in increasing order of distance from the origin. Thus near $z = a_n$, we shall have

$$f(z) \sim \frac{b_n}{z - a_n}\,, \tag{5.147}$$

where the constant b_n characterises the "strength" of the pole. In fact b_n is known as the *residue* at the pole $z = a_n$.

Consider a circle C_p centred on $z = 0$ and with radius R_p chosen so that it encloses p of the poles. To avoid problems, we choose R_p so that it does not pass through any pole. Then the function

$$G_p(z) \equiv f(z) - \sum_{n=1}^{p} \frac{b_n}{z - a_n} \tag{5.148}$$

will be analytic within the circle, since we have explicitly arranged to subtract out all the poles (which we are assuming all to be of order 1). Using Cauchy's integral, we shall therefore have

$$G_p(z) = \frac{1}{2\pi\,\mathrm{i}} \oint_{C_p} \frac{G_p(\zeta)\,d\zeta}{\zeta - z} = \frac{1}{2\pi\,\mathrm{i}} \oint_{C_p} \frac{f(\zeta)\,d\zeta}{\zeta - z} - \frac{1}{2\pi\,\mathrm{i}} \sum_{n=1}^{p} b_n \oint_{C_p} \frac{d\zeta}{(\zeta - z)(\zeta - a_n)}\,. \tag{5.149}$$

Now, each term in the sum here integrates to zero. This is because the integrand is

$$\frac{1}{(\zeta - z)(\zeta - a_n)} = \frac{1}{z - a_n}\Big[\frac{1}{\zeta - z} - \frac{1}{\zeta - a_n}\Big] \tag{5.150}$$

The integral (over ζ) is taken around a contour that encloses both the simple pole at $\zeta = z$ and the simple pole at $\zeta = a_n$. We saw earlier, in the proof of Cauchy's integral formula, that a contour integral running anti-clockwise around a simple pole $c/(\zeta - \zeta_0)$ gives the answer $2\pi\, c\, \mathrm{i}$, and so the result of integrating (5.150) around our contour is $(2\pi\,\mathrm{i} - 2\pi\,\mathrm{i})/(z - a_n) = 0$. Thus we conclude that

$$G_p(z) = \frac{1}{2\pi\,\mathrm{i}} \oint_{C_p} \frac{f(\zeta)\, d\zeta}{\zeta - z}\,. \tag{5.151}$$

Now, consider a sequence of ever-larger circles C_p, enclosing larger and larger numbers of poles. This defines a sequence of functions $G_p(z)$ for increasing p, each of which is analytic within R_p. We want to show that $G_p(z)$ is bounded as p tends to infinity, which will allow us to invoke Liouville's theorem and deduce that $G_\infty(z) = \text{constant}$. By a now-familiar method of argument, we suppose that M_p is the maximum value that $|f(\zeta)|$ attains anywhere on the circular contour of radius R_p. Then from (5.151) we shall have

$$|G_p(z)| \le \frac{M_p\, R_p}{R_p - |z|}\,. \tag{5.152}$$

Consider first the case of a function f for which M_p is bounded in value as R_p goes to infinity. Then, we see from (5.152) that $|G_p(z)|$ is bounded as p goes to infinity. By Liouville's theorem, it follows that $G_\infty(z)$ must just be a constant, c. Thus in this case we have

$$f(z) = c + \sum_{n=1}^\infty \frac{b_n}{z - a_n}\,. \tag{5.153}$$

We are left with one undetermined constant, c. This can be fixed by looking at one special value of z, and then equating the two sides in (5.153). Suppose, for example, that $f(z)$ is analytic at $z = 0$. We can then determine c by setting $z = 0$:

$$f(0) = c - \sum_{n=1}^\infty \frac{b_n}{a_n}\,, \tag{5.154}$$

and then plugging the solution for c back into (5.153), giving

$$f(z) = f(0) + \sum_{n=1}^\infty \Big[\frac{b_n}{z - a_n} + \frac{b_n}{a_n}\Big]\,. \tag{5.155}$$

(If $f(z)$ happens to have a pole at $z = 0$, then we just choose some other special value of z instead, when solving for c.)

We obtained this result by assuming that $f(z)$ was bounded on the circle of radius R_p, as R_p was sent to infinity. Even if this is not the case, one can often construct a related function, for example $f(z)/z^k$ for some suitable integer k, which *is* bounded on the circle. With appropriate minor modifications, a formula like (5.155) can then be obtained.

An example is long overdue. Consider the function $f(z) = \tan z$. which is, of course $(\sin z)/\cos z$. Now we have

$$\begin{aligned} \sin z &= \sin(x + \mathrm{i}\, y) = \sin x\, \cosh y + \mathrm{i}\, \cos x\, \sinh y\,, \\ \cos z &= \cos(x + \mathrm{i}\, y) = \cos x\, \cosh y - \mathrm{i}\, \sin x\, \sinh y\,, \end{aligned} \tag{5.156}$$

where we have used the standard results that $\cos(\mathrm{i}\, y) = \cosh y$ and $\sin(\mathrm{i}\, y) = \mathrm{i}\, \sinh y$. Thus we have

$$\begin{aligned} |\sin z|^2 &= \sin^2 x\, \cosh^2 y + \cos^2 x\, \sinh^2 y = \sin^2 x + \sinh^2 y\,, \\ |\cos z|^2 &= \cos^2 x\, \cosh^2 y + \sin^2 x\, \sinh^2 y = \cos^2 x + \sinh^2 y\,. \end{aligned} \tag{5.157}$$

It is evident that $|\sin z|$ is finite for all finite z, and that therefore $\tan z$ can have poles only when $\cos z$ vanishes. From the second expression for $|\cos z|^2$ in (5.157), we see that this can happen only if $y = 0$ and $\cos x = 0$, i.e. at

$$z = (n + \tfrac{1}{2})\pi\,, \tag{5.158}$$

where n is an integer.

Near $z = (n + \frac{1}{2})\pi$, say $z = \zeta + (n + \frac{1}{2})\pi$, where $|\zeta|$ is small, we shall have

$$\begin{aligned} \sin z &\longrightarrow \sin(n + \tfrac{1}{2})\pi = (-1)^n\,, \\ \cos z &\longrightarrow -\sin(n + \tfrac{1}{2})\pi\, \sin\zeta \longrightarrow -(-1)^n\, \zeta\,, \end{aligned} \tag{5.159}$$

and so the pole at $z = a_n = (n + \frac{1}{2})\pi$ has residue $b_n = -1$.

We also need to examine the boundedness of $f(z) = \tan z$ on the circles R_p. These circles are most conveniently taken to go precisely half way between the poles, so we should take $R_p = p\,\pi$. Now from (5.157) we have

$$|\tan z|^2 = \frac{\sin^2 x\, \cosh^2 y + \cos^2 x\, \sinh^2 y}{\cos^2 x\, \cosh^2 y + \sin^2 x\, \sinh^2 y} = \frac{\sin^2 x + \sinh^2 y}{\cos^2 x + \sinh^2 y}\,. \tag{5.160}$$

Bearing in mind that $\sin x$ and $\cos x$ are bounded by 1, that $\cos p\pi = (-1)^p \neq 0$, and that $\sinh^2 y$ and $\cosh^2 y$ both diverge like $\frac{1}{4} e^{2|y|}$ as $|y|$ tends to infinity, we see that $|\tan z|$ is indeed bounded on the circles R_p of radius $p\,\pi$, as p tends to infinity. Thus we can now invoke our result (5.155), to deduce that

$$\tan z = -\sum_{n=-\infty}^{\infty} \Big[\frac{1}{z-(n+\frac{1}{2})\,\pi} + \frac{1}{(n+\frac{1}{2})\pi)} \Big] \,. \tag{5.161}$$

We can split the summation range into the poles at positive and at negative values of x, by using

$$\sum_{n=-\infty}^{\infty} u_n = \sum_{n=0}^{\infty} u_n + \sum_{n=0}^{\infty} u_{-n-1}\,.\,, \tag{5.162}$$

Thus (5.161) gives

$$\tan z = -\sum_{n=0}^{\infty} \Big[\frac{1}{z-(n+\frac{1}{2})\,\pi} + \frac{1}{(n+\frac{1}{2})\pi)} \Big] - \sum_{n=0}^{\infty} \Big[\frac{1}{z+(n+\frac{1}{2})\,\pi} - \frac{1}{(n+\frac{1}{2})\pi)} \Big] \tag{5.163}$$

which, grouping the summands together, becomes

$$\tan z = \sum_{n=0}^{\infty} \frac{2z}{(n+\frac{1}{2})^2\,\pi^2 - z^2}\,. \tag{5.164}$$

This gives our series for the function $f(z) = \tan z$. Note that it displays the expected poles at all the places where the $\cos z$ denominator vanishes, namely at $z = (m+\frac{1}{2})\,\pi$, where m is any integer.

Another application of the result (5.155) is to obtain an expansion of an *entire function* as an infinite product. Suppose $f(z)$ is entire, meaning that it is analytic everywhere except at infinity. It follows that $f'(z)$ is an analytic function too, and so the function

$$g(z) \equiv \frac{f'(z)}{f(z)} = \frac{d}{dz}\,\log f(z) \tag{5.165}$$

is meromorphic for all finite z. (Its only singularities are poles at the places where $f(z)$ vanishes, i.e. at the *zeros* of $f(z)$.)

Let us suppose that $f(z)$ has only *simple* zeros, i.e. it vanishes like $c_n\,(z-a_n)$ near the zero at $z = a_n$, and furthermore, suppose that $f(0) \ne 0$. Thus we can apply the formula (5.155) to $g(z)$, implying that

$$\frac{d}{dz}\,\log f(z) = \frac{f'(0)}{f(0)} + \sum_{n=1}^{\infty} \Big[\frac{1}{z-a_n} + \frac{1}{a_n} \Big] \,. \tag{5.166}$$

This can be integrated to give

$$\log f(z) = \log f(0) + \frac{f'(0)}{f(0}\,z + \sum_{n=1}^{\infty} \Big[\log\Big(1-\frac{z}{a_n}\Big) + \frac{z}{a_n} \Big] \,. \tag{5.167}$$

Finally, exponentiating this, we get

$$f(z) = f(0)\, e^{[f'(0)/f(0)]\, z} \prod_{n=1}^{\infty} \Big(1 - \frac{z}{a_n}\Big)\, e^{z/a_n}\,. \tag{5.168}$$

This infinite-product expansion is valid for any entire function $f(z)$ with simple zeros at $z = a_n$, none of which is located at $z = 0$, whose logarithmic derivative f'/f is bounded on a set of circles R_p. Obviously, without too much trouble, generalisations can be obtained where some of these restrictions are removed.

Let us apply this result in an example. Consider the function $\sin z$. From (5.157) we see that it has zeros only at $y = 0$, $x = n\,\pi$. The zero at $z = 0$ is unfortunate, since in the derivation of (5.168) we required our entire function $f(z)$ to be non-zero at $z = 0$. But this is easily handled, by taking our entire function to be $f(z) = (\sin z)/z$, which tends to 1 at $z = 0$. We now have a function that satisfies all the requirements, and so from (5.168) we shall have

$$\frac{\sin z}{z} = \prod_{n=-\infty}^{\infty} \Big(1 - \frac{z}{n\,\pi}\Big)\, e^{\frac{z}{n\,\pi}}\,, \tag{5.169}$$

where the term $n = 0$ in the product is to be omitted. Combining the positive-n and negative-n terms pairwise, we therefore find that

$$\sin z = z \prod_{n=1}^{\infty} \Big[1 - \Big(\frac{z}{n\,\pi}\Big)^2\Big]\,. \tag{5.170}$$

It is manifest that this has zeros in all the right places.

5.4.3 Branch Points, and Many-valued Functions

All the functions we have considered so far have been single-valued ones; given a point z, the function $f(z)$ has a unique value. Many functions do not enjoy this property. A classic example is the function $f(z) = z^{1/2}$. This can take two possible values for each non-zero point z, for the usual reason that there is an ambiguity of sign in taking the square root. This can be made more precise here, by considering the representation of the point z as $z = r\, e^{\mathrm{i}\theta}$. Thus we shall have

$$f(z) = (r\, e^{\mathrm{i}\theta})^{\frac{1}{2}} = r^{\frac{1}{2}}\, e^{\frac{\mathrm{i}}{2}\,\theta}\,. \tag{5.171}$$

But we can also write $z = r\, e^{\mathrm{i}(\theta+2\pi)}$, since θ is periodic, with period 2π, on the complex plane. Now we obtain

$$f(z) = (r\, e^{\mathrm{i}\,(\theta+2\pi)})^{\frac{1}{2}} = r^{\frac{1}{2}}\, e^{\frac{\mathrm{i}}{2}\,\theta + \mathrm{i}\,\pi} = -r^{\frac{1}{2}}\, e^{\frac{\mathrm{i}}{2}\,\theta}\,. \tag{5.172}$$

In fact, if we look at the value of $f(z) = z^{1/2}$ on the circle $z = r\, e^{\mathrm{i}\,\theta}$, taking θ from $\theta = 0$ to $\theta_0 = 2\pi - \epsilon$, where ϵ is a small positive constant, we see that

$$f(r\, e^{\mathrm{i}\,\theta}) \longrightarrow -f(r)\,, \tag{5.173}$$

as θ approaches θ_0. But since we are back essentially to where we started in the complex plane, it follows that $f(z)$ must be *discontinuous*; it undergoes a jump in its value, on completing a circuit around the origin.

Of course although in this description we seemed to attach a particular significance to the positive real axis there is not really anything especially distinguished about this line. We could just as well have re-oriented our discussion, and concluded that the jump in the value of $f(z) = z^{1/2}$ occurred on some other axis emanating from the origin. The important invariant statement is that if you trace around any closed path that encircles the origin, the value of $z^{1/2}$ will have changed, by an overall factor of (-1), on returning to the starting point. The function $f(z) = z^{1/2}$ is double-valued on the complex plane.

If we continue on and take a second trip around the closed path, we will return again with a factor of (-1) relative to the previous visitation of the starting point. So after two rotations, we are back where we started and the function $f(z) = z^{1/2}$ is back to its original value too. This is expressed mathematically by the fact that

$$f(r\, e^{\mathrm{i}\,(\theta+4\pi)}) = r^{\frac{1}{2}}\, e^{\frac{\mathrm{i}}{2}\,\theta}\, e^{2\pi\,\mathrm{i}} = r^{\frac{1}{2}}\, e^{\frac{\mathrm{i}}{2}\,\theta} = f(r\, e^{\mathrm{i}\,\theta})\,. \tag{5.174}$$

An elegant way to deal with a multi-valued function such as $f(z) = z^{1/2}$ is to consider an enlarged two-dimensional surface on which the function is defined. In the case of the double-valued function $f(z) = z^{1/2}$, we can do it as follows. Imagine taking the complex plane, and making a semi-infinite cut along the real axis, from $x = 0$ to $x = +\infty$. Now, stack a second copy of the complex plane above this one, again with a cut from $x = 0$ to $x = +\infty$. Now, identify (i.e. glue) the lower edge of the cut of the underneath complex plane with the upper edge of the cut of the complex plane that sits on top. Finally (a little trickier to imagine!), identify the lower cut edge of the complex plane on top with the upper cut edge of the complex plane that sits underneath. We have created something a bit like a multi-story car-park (with two levels, in this case). As you drive anti-clockwise around the origin, starting on the lower floor, you find, after one circuit, that you have driven up onto the upper floor. Carrying on for one more circuit, you are back on the lower floor again.[21] What has been achieved is the creation of a two-sheeted surface, called a *Riemann*

[21] Of course multi-story car-parks don't work quite like that in real life, owing to the need to be able to embed them in three dimensions!

Surface, on which one has to take z around the origin through a total phase of 4π before before it returns to its starting point. The function $f(z) = z^{1/2}$ is therefore single-valued on this two-sheeted surface. "Ordinary" functions, i.e. ones that were single-valued on the original complex plane, simply have the property of taking the same value on each of the two sheets, at $z = r\, e^{\mathrm{i}\,\theta}$ and $z = r\, e^{\mathrm{i}\,(\theta+2\pi)}$.

We already noted that the choice of where to run the cut was arbitrary. The important thing is that for the function $f(z) = z^{1/2}$, it must run from $z = 0$ out to $z = \infty$, along any arbitrarily specifiable path. It is often convenient to take this to be the cut along the real positive axis, but any other choice will do.

The reason why the origin is so important here is that it is at $z = 0$ that the actual branch point of the function $f(z) = z^{1/2}$ lies. It is easy to see this, by following the value of $f(z) = z^{1/2}$ as z is taken around various closed paths (it is simplest to choose circles) in the complex plane. One easily sees that the $f(z) \longrightarrow -f(z)$ discontinuity is encountered for any path that encloses the origin, but no discontinuity arises for any closed path that does not enclose the origin.

If one encircles the origin, one also encircles the point at infinity, so $f(z) = z^{1/2}$ also has a branch point at infinity. (Clearly $f(1/\zeta) = \zeta^{-1/2}$ is also double valued on going around $\zeta = 0$.) So in fact, the *branch cut* that we must introduce is running from one branch point to the other. This is a general feature of multi-valued functions. In more complicated cases, this can mean that there are various possible choices for how to select the branch cuts. In the present case, choosing the branch cut along any arbitrary path from $z = 0$ to $z = \infty$ will do. Then, as one follows around a closed path, there is a discontinuity in $f(z)$ each time the branch cut is crossed. If a closed path crosses it twice (in opposite directions), then the two cancel out, and the function returns to its original value without any discontinuity.[22]

Consider another example, namely the function

$$f(z) = (z^2 - 1)^{\frac{1}{2}} = (z-1)^{\frac{1}{2}}\,(z+1)^{\frac{1}{2}}\,. \tag{5.175}$$

It is easy to see that since $z^{1/2}$ has a branch point at $z = 0$, here we shall have branch points at $z = 1$ and $z = -1$. Any closed path encircling either $z = -1$ or $z = +1$ (but not

[22] In the special case of $z^{1/2}$, for which the function is exactly two-valued, then crossing over the cut twice even both in the *same* direction will cause a cancellation of the discontinuity. But more generally, a double crossing of the branch will cause the discontinuities to cancel only if the crossings are in *opposite* directions. Of course *multiple* crossings of the cut in the same direction might lead to a cancellation, if the function is only finitely-many valued. For example, $f(z) = z^{1/n}$ is n-valued, so winding n times around in the same direction gets back to the original value, if n is an integer. On the other hand $f(z) = z^{1/\pi}$ will never return to its original value, no matter how many complete circuits of the origin are made.

both) will reveal a discontinuity associated with the two-valuedness of $(z+1)^{\frac{1}{2}}$ or $(z-1)^{\frac{1}{2}}$ respectively. On the other hand, a circuit that encloses *both* of the points $z=1$ and $z=-1$ will not encounter any discontinuity. The minus sign coming from encircling one branch point is cancelled by that coming from encircling the other. The upshot is that we can choose our branch cuts in either of two superficially-different ways. One of the choices is to run the branch cut from $z=-1$ to $z=+1$. Another quite different-looking choice is to run a branch cut from $z=1$ to $z=+\infty$ along the real positive axis, and another cut from $z=-1$ to $z=-\infty$ along the real negative axis.

For either of these choices, one gets the right conclusion. Namely, as one follows along any path, there is a discontinuity whenever a branch cut is crossed. Crossing twice in a given path will cause the two discontinuities to cancel out. so even if consider the second choice of branch cuts, with two cuts running out to infinity from the points $z=-1$ and $z=+1$, we get the correct conclusion that a closed path that encircles both $z=-1$ and $z=+1$ will reveal no discontinuity after returning to its starting point.

Actually the two apparently-different choices for the branch cuts are not so very different, topologically-speaking. Really, $z=\infty$ is like a single point, and one effectively should view the complex plane as the surface of a sphere, with everywhere out at infinity corresponding to the same point on the sphere. Think of making a stereographic projection from the north pole of the sphere onto the infinite plane tangent to the south pole. We think of this plane as the complex plane. A straight line joining the north pole to a given point in the complex plane therefore passes through a single point on the sphere. This gives a mapping from each point in the complex plane into a point on the sphere. Clearly, things get a bit degenerate as we go further and further out in the complex plane. Eventually, we find that all points at $|z|=\infty$, regardless of their direction out from the origin, map onto a single point on the sphere, namely the north pole. This sphere, known as the *Riemann Sphere*, is really what the complex plane is like. Of course as we have seen, a lot of otherwise well-behaved functions tend to have more severe singularities at $z=\infty$, but that doesn't detract from the usefulness of the picture. Figure 2 below show the mapping of a point Q in the complex plane into a corresponding point P on the Riemann sphere.

As it happens, our function $f(z)=(z^2-1)^{1/2}$ is rather moderately behaved at $z=\infty$; it has a Laurent expansion with just a simple pole:

$$\begin{aligned} f(1/\zeta) &= (\zeta^{-2}-1)^{\frac{1}{2}} = \zeta^{-1}\,(1-\zeta^2)^{\frac{1}{2}}\,,\\ &= \frac{1}{\zeta} - \tfrac{1}{2}\zeta - \tfrac{1}{8}\zeta^3 - \tfrac{1}{16}\,\zeta^5 + \cdots\,. \end{aligned} \tag{5.176}$$

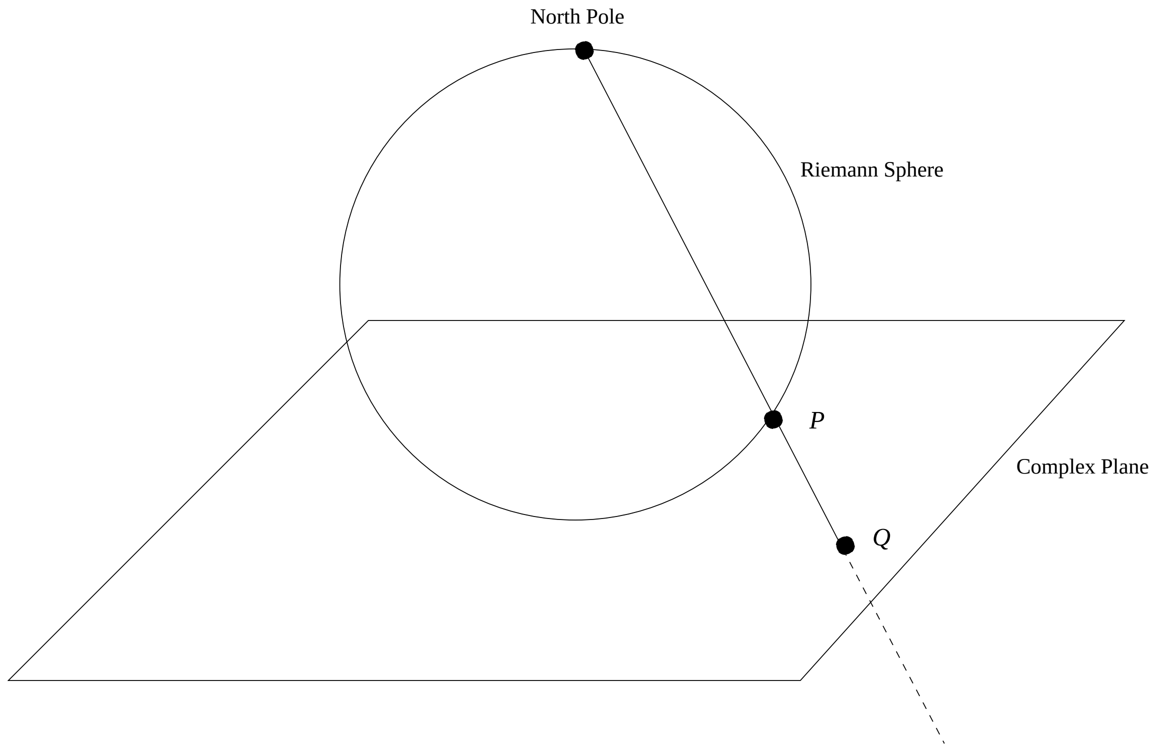

Figure 2: The point Q in the complex plane projects onto P on the Riemann sphere.

Since it has no branch point there, we can actually take the second choice of branch cuts, where the two cuts ran from $z = -1$ and $z = +1$ to infinity (in other words a single line from $z = -1$ to the north pole and back to $z = +1$), and deform it continuously into the first choice, where the branch cut simply runs from $z = -1$ to $z = +1$. If you think of the branch cut as an elastic band joining $z = -1$ to $z = +1$ via the north pole, it only takes someone like Superman wandering around at the north pole to give it a little tweak, and it can contract smoothly and continuously from the second choice of branch cut to the first.

5.5 The Oppenheim Formula

Before proceeding with the mainstream of the development, let us pause for an interlude on a rather elegant and curious topic. It is a rather little-known method for solving the following problem. Suppose we are given the real part $u(x, y)$ of an analytic function $f(z) = u(x, y) + \mathrm{i}\, v(x, y)$. It is a classic exercise, to work out the imaginary part $v(x, y)$, and hence to learn what the full analytic function $f(z)$ is, by making use of the Cauchy-Riemann equations.

Let us first consider this standard way to solve the problem. Before trying to solve for $v(x, y)$, it is worth checking to be sure that a solution exists. In other words, we can first verify that $u(x,y)$ is indeed the real part of an analytic function. We know that if it is, then the Cauchy-Riemann equations (5.57) must hold. As we saw earlier, these equations, $u_x = v_y$, $u_y = -v_x$, imply in particular that $u_{xx} + u_{yy} = 0$; i.e. that u satisfies the two-dimensional Laplace equation. In fact the implication goes in the other direction too; if $u(x,y)$ satisfies the Laplace equation $u_{xx} + u_{yy} = 0$ then it follows that it can be taken to be the real part of some analytic function. We can say that $u_{xx}+u_{yy} = 0$ is the *integrability condition* for the pair of equations $u_x = v_y$, $u_y = -v_x$ to admit a solution for $v(x,y)$.

To solve for $v(x,y)$ by the traditional method, one differentates $u(x,y)$ with respect to x or y, and integrates with respect to y or x respectively, to construct the function $v(x,y)$ using (5.57):

$$\begin{aligned} v(x,y) &= \int_{y_0}^{y} \frac{\partial u(x,y')}{\partial x}\, dy' + \alpha(x)\,, \\ v(x,y) &= -\int_{x_0}^{x} \frac{\partial u(x',y)}{\partial y}\, dx' + \beta(y)\,. \end{aligned} \tag{5.177}$$

The first integral, which comes from integrating $u_x = v_y$, leaves an arbitrary function of x unresolved, while the second, coming from integrating $u_y = -v_x$, leaves an arbitrary function of y unresolved. Consistency between the two resolves everything, up to an additive constant in $v(x,y)$. This constant never can be determined purely from the given data, since clearly if $f(z)$ is analytic then so is $f(z)+\mathrm{i}\,\gamma$, where γ is a real constant. But the real parts of $f(z)$ and $f(z)+\mathrm{i}\,\gamma$ are identical, and so clearly we cannot deduce the value of γ, merely from the given $u(x,y)$. Note that we do need both equations in (5.177), in order to determine $v(x,y)$ up to the additive constant γ. Of course the freedom to pick different constant lower limits of integration y_0 and x_0 in (5.177) just amounts to changing the arbitrary functions $\alpha(x)$ and $\beta(y)$, so we can choose y_0 and x_0 in any way we wish.

Let us check this with an example. Suppose we are given $u(x,y) = e^x \cos y$, and asked to find $v(x,y)$. A quick check shows that $u_{xx} + u_{yy} = 0$, so we will not be wasting our time by searching for $v(x,y)$. We have

$$u_x = v_y = e^x \cos y\,, \qquad u_y = -v_x = -e^x \sin y\,, \tag{5.178}$$

and so integrating as in (5.177) we get

$$v(x,y) = e^x \sin y + \alpha(x)\,, \qquad v(x,y) = e^x \sin y + \beta(y)\,. \tag{5.179}$$

Sure enough, the two expressions are compatible, and we see that $\alpha(x) = \beta(y)$. By the standard argument that is the same as one uses in the separation of variables, it must be that $\alpha(x) = \beta(y) = \gamma$, where γ is a (real) constant. Thus we have found that $v(x,y) = e^x \sin y + \gamma$, and so

$$
\begin{aligned}
f(z) &= u + \mathrm{i}\, v = e^x (\cos x + \mathrm{i} \sin y) + \mathrm{i}\,\gamma = e^x\, e^{\mathrm{i}\, y} + \mathrm{i}\,\gamma = e^{x + \mathrm{i}\, y} + \mathrm{i}\,\gamma \\
&= e^z + \mathrm{i}\,\gamma\,. \qquad (5.180)
\end{aligned}
$$

What is not so well known is that one can do the job of finding $v(x,y)$ from $u(x,y)$ without ever needing to differentiate or integrate at all. This makes a nice party trick, if you go to the right (or maybe wrong!) sort of parties. The way it works is absurdly simple, and so, in the best traditions of a conjuring trick, here first is the "show." Unlike the conjuror's trick, however, we shall see afterwards how the rabbit was slipped into the hat. I have not been able to find very full references to it; the earliest I came across is to a certain Prof. A. Oppenheim, so I shall refer to it as the "Oppenheim Method."

The way to derive the analytic function $f(z)$, given its real part $u(x,y)$, is the following:

$$
f(z) = 2u\Big(\frac{z}{2}, \frac{z}{2\,\mathrm{i}}\Big) + c\,, \qquad (5.181)
$$

where c is a constant. The real part of c can be fixed by using the known given expression for the real part of $f(z)$. The imaginary part of c is not determinable. Of course this is always the case; $f(z)$ and $f(z) + \mathrm{i}\,\gamma$, where γ is a real constant, have the same real parts and the same analyticity properties, so *no* method could tell us what γ is, in the absence of further specification. (In the usual Cauchy-Riemann derivation of $v(x,y)$, this arbitrariness arose as a constant of integration.)

Just to show that it really does work, consider the same example that we treated above using the traditional method. Suppose we are given that $u(x,y) = e^x \cos y$ is the real part of an analytic function $f(z)$. What is $f(z)$? According to (5.181), the answer is

$$
\begin{aligned}
f(z) &= 2e^{\frac{1}{2}z} \cos\Big(-\frac{\mathrm{i}}{2}\, z\Big) + c = 2e^{\frac{1}{2}z} \cosh\Big(\frac{1}{2} z\Big) + c\,, \\
&= e^z + 1 + c\,. \qquad (5.182)
\end{aligned}
$$

Now, we fix c by noting, for example, that from the original $u(x,y)$ we have $u(0,0) = 1$, and so we should choose c so that $f(z)$ has real part 1 at $z = 0$. Thus we have $c = -1$, and hence $f(z) = e^z$. (There is no need to be tedious about always adding $\mathrm{i}\,\gamma$, since this trivial point about the arbitrariness over the imaginary constant is now well understood.) Finally, we can easily verify that indeed $f(z) = e^z$ is the answer we were looking for, since

$$
e^z = e^{x + \mathrm{i}\, y} = e^x (\cos y + \mathrm{i} \sin y)\,, \qquad (5.183)
$$

and so sure enough, this analytic function has real part $e^x \cos y$.

How did it work? Like all the best conjuring tricks, the explanation is ludicrously simple. Since $f(z)$ is analytic, we can expand it as a power series, $f(z) = \sum_{n\ge 0} a_n\, z^n$. Note that we are assuming here that it is in particular analytic at $z = 0$; we shall show later how to remove this assumption. If we write the expansion coefficients a_n as $a_n = \alpha_n + \mathrm{i}\,\beta_n$, where α_n and β_n are real, then from the series expansion we shall have

$$2u(x,y) = f(z) + \overline{f(z)} = \sum_{n\ge 0} \Big[(\alpha_n + \mathrm{i}\,\beta_n)\,(x+\mathrm{i}\,y)^n + (\alpha_n - \mathrm{i}\,\beta_n)\,(x-\mathrm{i}\,y)^n\Big]\,. \tag{5.184}$$

Now plug in the values $x = z/2$, $y = z/(2\mathrm{i})$, as required in the Oppenheim formula:

$$\begin{aligned} 2u(\frac{z}{2},\frac{z}{2\mathrm{i}}) &= \sum_{n\ge 0} \Big[(\alpha_n + \mathrm{i}\,\beta_n)\Big(\frac{z}{2}+\frac{z}{2}\Big)^n + (\alpha_n - \mathrm{i}\,\beta_n)\Big(\frac{z}{2}-\frac{z}{2}\Big)^n\Big]\,, & (5.185)\\ nn &= \sum_{n\ge 0}(\alpha_n + \mathrm{i}\,\beta_n)\,z^n + \alpha_0 - \mathrm{i}\,\beta_0\,, & (5.186)\\ &= f(z) + \alpha_0 - \mathrm{i}\,\beta_0\,. \end{aligned}$$

That's all there is to it! The result is proven. *Omne ignotum pro magnifico.*

We assumed in the proof that $f(z)$ was analytic at $z = 0$. If it's not, then in its present form the procedure can sometimes break down. For example, suppose we consider the function $u(x,y) = \frac{1}{2}\log(x^2+y^2)$. (Secretly, we know that this is the real part of the function $f(z) = \log z$, which of course is analytic for all finite z except for the branch point at $z = 0$.) Trying the Oppenheim formula (5.181), we get

$$f(z) = \log(\frac{1}{4}z^2 - \frac{1}{4}z^2) + c = \log 0 + c\,. \tag{5.187}$$

Oooppps!! Not to worry, we know why it has failed. We need to find a generalisation of the Oppenheim formula, to allow for such cases where the function we are looking for happens to be non-analytic at $z = 0$. The answer is the following:

$$f(z) = 2u(\frac{z+a}{2},\frac{z-a}{2\mathrm{i}}) + c\,, \tag{5.188}$$

where a is an arbitrary constant, to be chosen to avoid any unpleasantness. Let's try this in our function $u(x,y) = \frac{1}{2}\log(x^2+y^2)$:

$$\begin{aligned} f(z) &= \log\Big[\Big(\frac{z+a}{2}\Big)^2 - \Big(\frac{z-a}{2}\Big)^2\Big] + c\,,\\ &= \log(a\,z) + c = \log z + \log a + c\,. & (5.189)\end{aligned}$$

So for any value of a other than $a = 0$, everything is fine. As usual, an elementary examination of a special case fixes the real part of the constant c, to give $c = -\log a$.

It is easy to see why the generalisation (5.188) works. We just repeat the derivation in (5.186), but now consider an expansion of the function $f(z)$ around $z = a$ rather than $z = 0$; $f(z) = \sum_{n\ge 0} a_n\,(z-a)^n$. Provided we don't choose a so that we are trying to expand around a singular point of $f(z)$, all must then be well:

$$
\begin{aligned}
2u(\frac{z+a}{2},\frac{z-a}{2\mathrm{i}}) &= \sum_{n\ge 0}\Big[(\alpha_n+\mathrm{i}\,\beta_n)\Big(\frac{z+a}{2}+\frac{z-a}{2}-a\Big)^n+(\alpha_n-\mathrm{i}\,\beta_n)\Big(\frac{z+a}{2}-\frac{z-a}{2}-a\Big)^n\Big]\,,\\
&= \sum_{n\ge 0}(\alpha_n+\mathrm{i}\,\beta_n)\,(z-a)^n+\alpha_0-\mathrm{i}\,\beta_0\,, \qquad (5.190)\\
&= f(z)+\alpha_0-\mathrm{i}\,\beta_0\,.
\end{aligned}
$$

Just to show off the method in one further example, suppose we are given

$$
u(x,y)=e^{\frac{x}{x^2+y^2}}\,\cos\frac{y}{x^2+y^2}\,. \qquad (5.191)
$$

Obviously we shall have to use (5.188) with $a\ne 0$ here. Thus we get

$$
\begin{aligned}
f(z) &= 2e^{\frac{z+a}{2a\,z}}\,\cos\frac{z-a}{2\mathrm{i}\,a\,z}+c=2e^{\frac{z+a}{2a\,z}}\,\cosh\frac{z-a}{2a\,z}\,,\\
&= e^{\frac{z+a}{2a\,z}}\Big(e^{\frac{z-a}{2a\,z}}+e^{\frac{a-z}{2a\,z}}\Big)+c\,, \qquad (5.192)\\
&= e^{\frac{1}{a}}+e^{\frac{1}{z}}+c\,.
\end{aligned}
$$

Fixing the constant c from a special case, we get

$$
f(z)=e^{\frac{1}{z}}\,. \qquad (5.193)
$$

The method has even worked for a function with an essential singularity, provided that we take care not to try using $a = 0$. (Try doing the calculation by the traditional procedure using (5.177) to see how much simpler it is to use the generalised Oppenheim formula.)

Having shown how effective the Oppenheim method is, it is perhaps now time to admit to why in some sense a little bit of a cheat is being played here. This is not to say that anything was incorrect; all the formulae derived are perfectly valid. It is a slightly unusual kind of trick that has been played, in fact.

Normally, when a conjuror performs a trick, it is he who "slips the rabbit into the hat," and then pulls it out at the appropriate moment to astound his audience. Ironically enough, in the case of the Oppenheim formula it is the audience itself that unwittingly slips the rabbit into the hat, and yet nevertheless it is duly amazed when the rabbit reappears.

The key point is that if one were actually working with a realistic problem, in which only the real part of an analytic function were known, one would typically be restricted to knowing it only as an "experimental result" from a set of observations. Indeed, in a common circumstance such information about the real part of an analytic function might arise precisely from an experimental observation of, for example, the refractive index of a medium as a function of frequency. The *imaginary part*, on the other hand, is related to the decay of the wave as it moves through the medium. There are quite profound *Dispersion Relations* that can be derived that relate the imaginary part to the real part. They are derived precisely by making use of the Cauchy-Riemann relations, to derive $v(x, y)$ from $u(x, y)$ by taking the appropriate derivatives and integrals of $u(x, y)$, as in (5.177).

So why was the Oppenheim formula a cheat? The answer is that it assumes that one knows what happens if one inserts complex values like $x = (z + a)/2$ and $y = (z - a)/(2\mathrm{i})$ into the "slots" of $u(x, y)$ that are designed to take the real numbers x and y. In a real-life experiment one cannot do this; one cannot set the frequency of a laser to a complex value! So the knowledge about the function $u(x, y)$ that the Oppenheim formula requires one to have is knowledge that is not available in practical situations. In those real-life cases, one would instead have to use (5.177) to calculate $v(x, y)$. And the process of integration is "non-local," in the sense that the value for the integral depends upon the values that the integrand takes in an entire region in the (x, y) plane. This is why dispersion relations actually contain quite subtle information.

The ironic thing is that although the Opennheim formula is therefore in some sense a "cheat," it nevertheless works, and works correctly, in any example that one is likely to check it with. The point is that when we want to test a formula like that, we tend not to go out and start measuring refractive indices; rather, we reach into our memories and drag out some familiar function whose properties have already been established. So it is a formula that is "almost never" usable, and yet it works "almost always" when it is tested with toy examples. It is a bit like asking someone to pick a random number. Amongst the set of all numbers, the chance that an arbitrarily chosen number will be rational is zero, and yet the chance that the person's chosen number will be rational is pretty close to unity.

5.6 Calculus of Residues

After some rather lengthy preliminaries, we have now established the groundwork for the further development of the subject of complex integration. First, we shall derive a general result about the integration of functions with poles.

If $f(z)$ has an isolated pole of order n at $z = a$, then by definition, it can be expressed as

$$f(z) = \frac{a_{-n}}{(z-a)^n} + \frac{a_{-n+1}}{(z-a)^{n-1}} + \cdots + \frac{a_{-1}}{z-a} + \phi(z)\,, \tag{5.194}$$

where $\phi(z)$ is analytic at and near $z = a$. The coefficient of a_{-1} in this expansion is called the *residue* of $f(z)$ at the pole at $z = a$.

Let us consider the integral of $f(z)$ around a closed contour C which encloses the pole at $z = a$, but within which $\phi(z)$ is analytic. (So C encloses no other singularities of $f(z)$ except the pole at $z = a$.) We have

$$\oint_C f(z)\, dz = \sum_{k=1}^{n} a_{-k} \oint_C \frac{dz}{(z-a)^k} + \oint \phi(z)\, dz\,. \tag{5.195}$$

By Cauchy's theorem we know that the last integral vanishes, since $\phi(z)$ is analytic within C. To evaluate the integrals under the summation, we may deform the contour C to a circle of radius ρ centred on $z = a$, respecting the previous condition that no other singularities of $f(z)$ shall be encompassed.

Letting $z - a = \rho\, e^{\mathrm{i}\theta}$, the deformed contour C is then parameterised by allowing θ to range from 0 to 2π, while holding ρ fixed. Thus we shall have

$$\oint_C \frac{dz}{(z-a)^k} = \int_0^{2\pi} \frac{\mathrm{i}\,\rho\, e^{\mathrm{i}\theta}\, d\theta}{\rho^k e^{\mathrm{i}\,k\,\theta}} = \mathrm{i}\,\rho^{1-k} \int_0^{2\pi} e^{(1-k)\,\mathrm{i}\,\theta}\, d\theta = \rho^{1-k} \Big[\frac{e^{(1-k)\,\mathrm{i}\,\theta}}{1-k}\Big]_0^{2\pi}\,. \tag{5.196}$$

When the integer k takes any value other than $k = 1$, this clearly gives zero. On the other hand, when $k = 1$ we have

$$\oint_C \frac{dz}{z-a} = \mathrm{i} \int_0^{2\pi} d\theta = 2\pi\,\mathrm{i} \tag{5.197}$$

as we saw when deriving Cauchy's integral formula. Thus we arrive at the conclusion that

$$\oint_C f(z)\, dz = 2\pi\,\mathrm{i}\, a_{-1}\,. \tag{5.198}$$

The result (5.198) gives the value of the integral when the contour C encloses only the pole in $f(z)$ located at $z = a$. Clearly, if the contour were to enclose several poles, at locations $z = a$, $z = b$, $z = c$, *etc.*, we could smoothly deform C so that it described circles around each of the poles, joined by narrow "causeways" of the kind that we encountered previously, which would contribute nothing to the total integral.

Thus we arrive at the *Theorem of Residues*, which asserts that if $f(z)$ be analytic everywhere within a contour C, except at a number of isolated poles inside the contour, then

$$\oint_C F(z)\, dz = 2\pi\,\mathrm{i} \sum_s \mathcal{R}_s\,, \tag{5.199}$$

where $\mathcal{R}_s$ denotes the residue at pole number s.

It is useful to note that if $f(z)$ has a simple pole at $z = a$, then the residue at $z = a$ is given by taking the limit of $(z-a)\, f(z)$ as z tends to a.

5.7 Evaluation of real integrals

The theorem of residues can be used in order to evaluate many kinds of integrals. Since this is an important application, we shall look at a number of examples. First, a list of three main types of real integral that we shall be able to evaluate:

(1) Integrals of the form

$$\int_0^{2\pi} R(\cos\theta, \sin\theta)\, d\theta\,, \tag{5.200}$$

where R is a rational function of $\cos\theta$ and $\sin\theta$. (Recall that if $f(z)$ is a *rational* function, it means that it is the ratio of two polynomials.)

(2) Integrals of the form

$$\int_{-\infty}^{\infty} f(x)\, dx\,, \tag{5.201}$$

where $f(z)$ is analytic in the upper half plane ($y > 0$) except for poles that do not lie on the real axis. The function $f(z)$ is also required to have the property that $z\, f(z)$ should tend to zero as $|z|$ tends to infinity whenever $0 \le \arg(z) \le \pi$. ($\arg(z)$ is the *phase* of z. This condition means that $z\, f(z)$ must go to zero for all points z that go to infinity in the upper half plane.)

(3) Integrals of the form

$$\int_0^{\infty} x^{\alpha-1}\, f(x)\, dx\,, \tag{5.202}$$

where $f(z)$ is a rational function, analytic at $z = 0$, with no poles on the positive real axis. Furthermore, $z^\alpha\, f(z)$ should tend to zero as z approaches 0 or infinity.

First, consider the type (1) integrals. We introduce z as the complex variable $z = e^{\mathrm{i}\,\theta}$. Thus we have

$$\cos\theta = \tfrac{1}{2}(z + z^{-1})\,, \qquad \sin\theta = \tfrac{1}{2\mathrm{i}}(z - z^{-1})\,. \tag{5.203}$$

Recalling that R is a rational function of $\cos\theta$ and $\sin\theta$, it follows that the integral (5.200) will become a contour integral of some rational function of z, integrated around a unit circle centred on the origin. It is a straightforward procedure to evaluate the residues of the poles in the rational function, and so, by using the theorem of residues, the result follows.

Let us consider an example. Suppose we wish to evaluate

$$I(p) \equiv \int_0^{2\pi} \frac{d\theta}{1 - 2p\, \cos\theta + p^2}\,, \tag{5.204}$$

where $0 < p < 1$. Writing $z = e^{\mathrm{i}\,\theta}$, we shall have $d\theta = -\mathrm{i}\, z^{-1}\, dz$, and hence

$$I(p) = \oint_C \frac{dz}{\mathrm{i}\,(1 - p\, z)(z - p)}\,. \tag{5.205}$$

This has simple poles, at $z = p$ and $z = 1/p$. Since we are assuming that $0 < p < 1$, it follows from the fact that C is the unit circle that the pole at $z = 1/p$ lies outside C, and so the only pole enclosed is the simple pole at $z = p$. Thus the residue of the integrand at $z = p$ is given by taking the limit of

$$(z - p)\Big[\frac{1}{\mathrm{i}\,(1 - p\, z)(z - p)}\Big] \tag{5.206}$$

as z tends to p, i.e. $-\mathrm{i}/(1 - p^2)$. Thus from the theorem of residues (5.199), we get

$$\int_0^{2\pi} \frac{d\theta}{1 - 2p\,\cos\theta + p^2} = \frac{2\pi}{1 - p^2}\,, \qquad 0 < p < 1\,. \tag{5.207}$$

Note that if we consider the same integral (5.204), but now take the constant p to be greater than 1, the contour C (the unit circle) now encloses only the simple pole at $z = 1/p$. Multiplying the integrand by $(z - 1/p)$, and taking the limit where z tends to $1/p$, we now find that the residue is $+\mathrm{i}/(1 - p^2)$, whence

$$\int_0^{2\pi} \frac{d\theta}{1 - 2p\,\cos\theta + p^2} = \frac{2\pi}{p^2 - 1}\,, \qquad p > 1\,. \tag{5.208}$$

In fact the results for all real p can be combined into the single formula

$$\int_0^{2\pi} \frac{d\theta}{1 - 2p\,\cos\theta + p^2} = \frac{2\pi}{|p^2 - 1|}\,. \tag{5.209}$$

For a more complicated example, consider

$$I(p) \equiv \int_0^{2\pi} \frac{\cos^2 3\theta\, d\theta}{1 - 2p\,\cos 2\theta + p^2}\,, \tag{5.210}$$

with $0 < p < 1$. Now, we have

$$I(p) = \oint_C \frac{\left(\frac{1}{2} z^3 + \frac{1}{2} z^{-3}\right)^2 dz}{\mathrm{i}\, z\,(1 - p\, z^2)(1 - p\, z^{-2})} = \oint_C \frac{(z^6 + 1)^2\, dz}{4\mathrm{i}\, z^5\,(1 - p\, z^2)(z^2 - p)}\,. \tag{5.211}$$

The integrand has poles at $z = 0$, $z = \pm p^{\frac{1}{2}}$ and $z = \pm p^{-\frac{1}{2}}$. Since we are assuming $0 < p < 1$, it follows that only the poles at $z = 0$ and $z = \pm p^{\frac{1}{2}}$ lie within the unit circle corresponding to the contour C. The poles at $z = \pm p^{\frac{1}{2}}$ are simple poles, and the only slight complication in this example is that the pole at $z = 0$ is of order 5, so we have to work a little harder to extract the residue there. Shortly, we shall derive a general formula that can sometimes be useful in such circumstances. An alternative approach, often in practise preferrable when one is working out the algebra by hand (as opposed to using an algebraic computing program), is simply to factor out the singular behaviour and then make a Taylor expansion of the remaining regular function, as we described earlier. In this case, it is quite simple. We have

$$\begin{aligned}\frac{(z^6+1)^2}{z^5\,(1-p\,z^2)(z^2-p)} &= -\frac{1}{p\,z^5}\,(1+z^6)^2\,(1-p\,z^2)^{-1}\,(1-z^2\,p^{-1})^{-1}\\ &= -\frac{1}{p\,z^5}\,(1+p\,z^2+p^2\,z^4+\cdots)(1+z^2\,p^{-1}+z^4\,p^{-2}+\cdots)\\ &= -\frac{1}{p\,z^5}\,(1+p\,z^2+p^2\,z^4+z^2\,p^{-1}+z^4+z^4\,p^{-2}+\cdots)\\ &= -\frac{1}{p\,z^5}-\frac{(p^2+1)}{p^2\,z^3}-\frac{(p^4+p^2+1)}{p^3\,z}+\cdots\,, \end{aligned} \tag{5.212}$$

from which we read off the residue of this function at $z=0$ as the coefficient of $1/z$. Notice that to make these expansions we just used $(1-x)^{-1}=1+x+x^2+\cdots$, and that we only needed to push these expansions far enough to collect the terms at order z^4 that are then multiplied by $1/z^5$.

After a little further algebra for the two simple poles, we find that the residues of the integrand in (5.211) at $z=0$, $z=p^{\frac{1}{2}}$ and $z=-p^{\frac{1}{2}}$ are given by

$$\frac{\mathrm{i}\,(1+p^2+p^4)}{4p^3}\,,\qquad -\frac{\mathrm{i}\,(1+p^3)^2}{8p^3\,(1-p^2)}\,,\qquad -\frac{\mathrm{i}\,(1+p^3)^2}{8p^3\,(1-p^2)}\,, \tag{5.213}$$

respectively. Plugging into the theorem of residues (5.199), we therefore obtain the result

$$\int_0^{2\pi}\frac{\cos^2 3\theta\,d\theta}{1-2p\,\cos 2\theta+p^2}=\frac{\pi\,(1-p+p^2)}{(1-p)}\,, \tag{5.214}$$

when $0<p<1$.

It is sometimes useful to have a general result for the evaluation of the residue at an n'th-order pole. It really just amounts to formalising the procedure we used above, of extracting the singular behaviour and then Taylor expanding the remaining analytic factor:

If $f(z)$ has a pole of order n at $z=a$, it follows that it will have the form

$$f(z)=\frac{g(z)}{(z-a)^n}\,, \tag{5.215}$$

where $g(z)$ is analytic in the neighbourhood of $z=a$. Thus we may expand $g(z)$ in a Taylor series around $z=a$, giving

$$\begin{aligned} f(z) &= \frac{1}{(z-a)^n}\Big(g(a)+(z-a)\,g'(a)+\cdots+\frac{1}{(n-1)!}\,(z-a)^{n-1}\,g^{(n-1)}(a)+\cdots\Big)\,,\\ &= \frac{g(a)}{(z-a)^n}+\frac{g'(a)}{(z-a)^{n-1}}+\cdots+\frac{g^{(n-1)}(a)}{(n-1)!\,(z-a)}+\cdots\,. \end{aligned} \tag{5.216}$$

We then read off the residue, namely the coefficient of the first-order pole term $1/(z-a)$, finding $g^{(n-1)}(a)/(n-1)!$. Re-expressing this in terms of the original function $f(z)$, using (5.215), we arrive at the general result that

If $f(z)$ has a pole of order n at $z = a$, then the residue $\mathcal{R}$ is given by

$$\mathcal{R} = \frac{1}{(n-1)!} \Big[\frac{d^{n-1}}{dz^{n-1}} \left((z-a)^n f(z)\right)\Big]_{z=a} . \tag{5.217}$$

It is straightforward to check that when applied to our example in (5.211), the formula (5.217) reproduces our previous result for the residue at the 5'th-order pole at $z = 0$. In practise, though, it is usually more convenient in a hand calculation to use the method described previously, rather than slogging out the derivatives needed for (5.217).

As a final example of the type (1) class of integrals, consider

$$I(a,b) \equiv \int_0^{2\pi} \frac{d\theta}{(a + b\,\cos\theta)^2} = \oint_C \frac{4z\,dz}{\mathrm{i}\,(b + 2a\,z + b\,z^2)^2} , \tag{5.218}$$

where $a > b > 0$. The integrand has (double) poles at

$$z = \frac{-a \pm \sqrt{a^2 - b^2}}{b} , \tag{5.219}$$

and so just the pole at $z = (-a + \sqrt{a^2 - b^2})/b$ lies inside the unit circle. After a little calculation, one finds the residue there, and hence, from (5.199), we get

$$\int_0^{2\pi} \frac{d\theta}{(a + b\,\cos\theta)^2} = \frac{2\pi\,a}{(a^2 - b^2)^{\frac{3}{2}}} . \tag{5.220}$$

Turning now to integrals of type 2 (5.201), the approach here is to consider a contour integral of the form

$$I \equiv \oint_C f(z)\,dz , \tag{5.221}$$

where the contour C is taken to consist of the line from $x = -R$ to $x = +R$ along the x axis, and then a semicircle of radius R in the upper half plane, thus altogether forming a closed path.

The condition that $z\,f(z)$ should go to zero as $|z|$ goes to infinity with $0 \le \arg(z) \le \pi$ ensures that the contribution from integrating along the semicircular arc will vanish when we send R to infinity. (On the arc we have $dz = \mathrm{i}\,R\,e^{\mathrm{i}\,\theta}\,d\theta$, and so we would like $R\,f(R\,e^{\mathrm{i}\,\theta})$ to tend to zero as R tends to infinity, for all θ in the range $0 \le \theta \le \pi$, whence the condition that we placed on $f(z)$.) Thus we shall have that

$$\int_{-\infty}^{\infty} f(x)\,dx = 2\pi\,\mathrm{i} \sum_s \mathcal{R}_s , \tag{5.222}$$

where the sum is taken over the residues $\mathcal{R}_s$ at all the poles of $f(z)$ in the upper half plane. The contour is depicted in Figure 3 below.

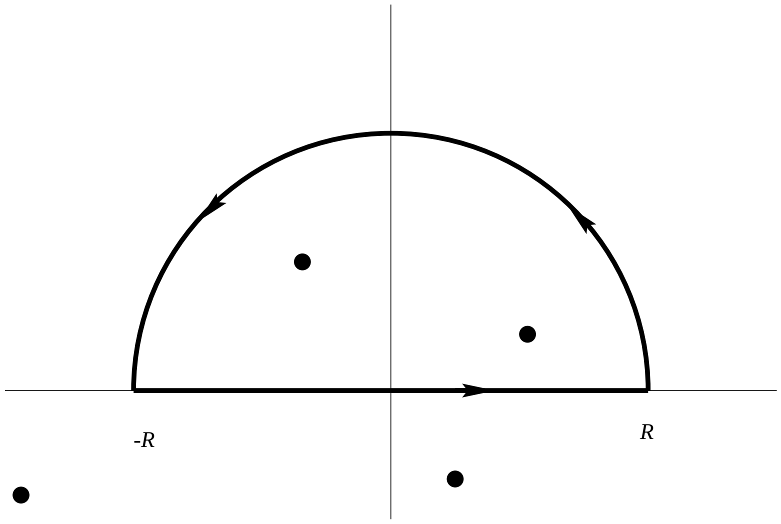

Figure 3: The contour encloses poles of $f(z)$ in the upper half plane

Consider, as a simple example,

$$\int_{-\infty}^{\infty} \frac{dx}{1+x^2} \,. \tag{5.223}$$

Clearly, the function $f(z) = (1+z^2)^{-1}$ fulfils all the requirements for this type of integral. Since $f(z) = (z+\mathrm{i})^{-1}\,(z-\mathrm{i})^{-1}$, we see that there is just a single pole in the upper half plane, at $z = \mathrm{i}$. It is a simple pole, and so the residue of $f(z)$ there is $1/(2\mathrm{i})$. Consequently, from (5.222) we derive

$$\int_{-\infty}^{\infty} \frac{dx}{1+x^2} = \pi \,. \tag{5.224}$$

Of course in this simple example we could perfectly well have evaluated the integral instead by more "elementary" means. A substitution $x = \tan\theta$ would convert (5.223) into

$$\int_{-\frac{1}{2}\pi}^{\frac{1}{2}\pi} d\theta = \pi \,. \tag{5.225}$$

However, in more complicated examples the contour integral approach is often much easier to use. Consider, for instance, the integral

$$\int_{-\infty}^{\infty} \frac{x^4\,dx}{(a+b\,x^2)^4} \,, \tag{5.226}$$

where $a > 0$ and $b > 0$. The function $f(z) = z^4\,(a+b\,z^2)^{-4}$ has poles of order 4 at $z = \pm\mathrm{i}(a/b)^{\frac{1}{2}}$, and so there is just one pole in the upper half plane. Using either the formula

(5.217), or the direct approach of extracting the singular factor and Taylor-expanding "by hand" to calculate the residue, and multiplying by $2\pi\,\mathrm{i}$, we get

$$\int_{-\infty}^{\infty} \frac{x^4\, dx}{(a+b\,x^2)^4} = \tfrac{1}{16}\,\pi\, a^{-\frac{3}{2}}\, b^{-\frac{5}{2}}\,. \tag{5.227}$$

Just to illustrate the point, we may note that we could in principle have worked out (5.226) by "elementary means," but the procedure would be quite unpleasant to implement. By means of an appropriate trigonometric substitution, one eventually concludes that the integral (5.226) gives

$$\int_{-\infty}^{\infty} \frac{x^4\, dx}{(a+b\,x^2)^4} = \Big[\frac{3b^2\,x^5 - 8a\,b\,x^3 - 3a^2\,x}{48a\,b^2\,(a+b\,x^2)^3} + \frac{1}{16a^{3/2}\,b^{5/2}}\,\arctan\Big(\frac{\sqrt{b}\,x}{\sqrt{a}}\Big)\Big]_{-\infty}^{\infty}\,, \tag{5.228}$$

from which the result (5.228) follows. If you try it, you will find that the labour involved is *much* more than in the contour integral method.

One reason for the great saving of labour when using the contour integral method is that when using the old-fashioned approach of first evaluating the indefinite integral, and then substituting the limits of integration, one is actually working out much more than is ever needed. It is intrinsically a more complicated exercise to find the function whose derivative is $f(x)$ than it is to find the result of integrating $f(x)$ over a fixed interval such as $-\infty$ to ∞. If we look at the first term in (5.227) (the rational function of x), we see that they disappear altogether when one sets x to its limiting values of $-\infty$ and $+\infty$. And yet by the old-fashioned method it is necessary first to thrash out the entire integral, including these terms, since we don't know in advance how to recognise that some of the terms in the final result will end up getting thrown away when the limits are substituted. In our example above, the indefinite integral *is* still doable, albeit with a struggle. In more complicated examples there may be no closed-form expression for the indefinite integral, and yet the definite integral may have a simple form, easily found by contour-integral methods.

Finally, consider integrals of type 3 (5.202). In general, α is assumed to be a real number, but not an integer. We consider the function $(-z)^{\alpha-1}\,f(z)$, which therefore has a branch-point singularity at $z=0$. We consider a contour C of exactly the form given in Figure 1, with $a=0$. Eventually, we allow the radius of the larger circle C_1 to become infinite, while the radius of the smaller circle C_2 will go to zero. In view of the assumption that $z^\alpha\,f(z)$ goes to zero as z goes to 0 or infinity, it follows that the contributions from integrating around these two circles will give zero.

Unlike the situation when we used the contour of Figure 1 for deriving the Laurent series, we are now faced with a function $(-z)^{\alpha-1}\,f(z)$ with a branch point at $z=0$. Consequently, there is a discontinuity as one traces the value of $(-z)^{\alpha-1}\, f(z)$ around a closed path that encircles the origin. This means that the results of integrating along the two sides of the "causeway" connecting the circles C_1 and C_2 will not cancel.

We can take the phase of $(-z)^{\alpha-1}$ to be *real* when z lies on the negative real axis, such as at the point where the small circle C_2 intersects the negative real axis. Consequently, on the *lower* part of the causeway (below the positive real axis), the phase will be $e^{i\pi\,(\alpha-1)}$. On the other hand, on the *upper* part of the causeway (above the positive real axis), the phase will be $e^{-i\pi\,(\alpha-1)}$. Thus we find that

$$\begin{aligned}\oint_C (-z)^{\alpha-1}\, f(z)\, dz &= -e^{i\pi\,(\alpha-1)} \int_0^\infty x^{\alpha-1}\, f(x)\, dx + e^{-i\pi\,(\alpha-1)} \int_0^\infty x^{\alpha-1}\, f(x)\, dx\,,\\ &= 2i\, \sin(\pi\,\alpha) \int_0^\infty x^{\alpha-1}\, f(x)\, dx\,,\end{aligned} \tag{5.229}$$

where the minus sign on the first term on the right in the top line comes from the fact that the integral from $x=0$ to $x=\infty$ is running in the direction opposite to the indicated direction of the contour in Figure 1. The contour integral on the left-hand side picks up all the contributions from the poles of $f(z)$. Thus we have the result that

$$\int_0^\infty x^{\alpha-1}\, f(x)\, dx = \frac{\pi}{\sin\pi\alpha} \sum_s \mathcal{R}_s\,, \tag{5.230}$$

where $\mathcal{R}_s$ is the residue of $(-z)^{\alpha-1}\, f(z)$ at pole number s of the function $f(z)$.

As an example, consider the integral

$$\int_0^\infty \frac{x^{\alpha-1}\, dx}{1+x}\,. \tag{5.231}$$

Here, we therefore have $f(z) = 1/(z+1)$, which just has a simple pole, at $z=-1$. The residue of $(-z)^{\alpha-1}\, f(z)$ is therefore just 1, and so from (5.230) we obtain that when $0 < \alpha < 1$,

$$\int_0^\infty \frac{x^{\alpha-1}\, dx}{1+x} = \frac{\pi}{\sin\pi\alpha}\,. \tag{5.232}$$

(The restriction $0 < \alpha < 1$ is to ensure that the fall-off conditions for type 3 integrands at $z=0$ and $z=\infty$ are satisfied.)

A common circumstance is when there is in fact a pole in the integrand that lies exactly on the path where we wish to run the contour. An example would be an integral of the type (2) discussed above, but where the integrand now has poles on the real axis. If these are *simple* poles, then the following method can be used. Consider a situation where we wish to evaluate $\int_{-\infty}^\infty f(x)\, dx$, and $f(z)$ has a single simple pole on the real axis, at $z=a$. What we do is to make a little detour in the contour, to skirt around the pole, so the contour C in

Figure 3 now aquires a little semicircular "bypass" γ, of radius ρ, taking it into the upper half plane around the point $z = a$. This is shown in Figure 4 below. Thus before we take the limit where $R \longrightarrow \infty$, we shall have

$$\int_{-R}^{a-\rho} f(x)\,dx + \int_\gamma f(z)\,dz + \int_{a+\rho}^{R} f(x)\,dx = 2\pi\,\mathrm{i} \sum_j \mathcal{R}_j\,, \tag{5.233}$$

where as usual $\mathcal{R}_j$ is the residue of $f(z)$ at its j'th pole in the upper half plane.

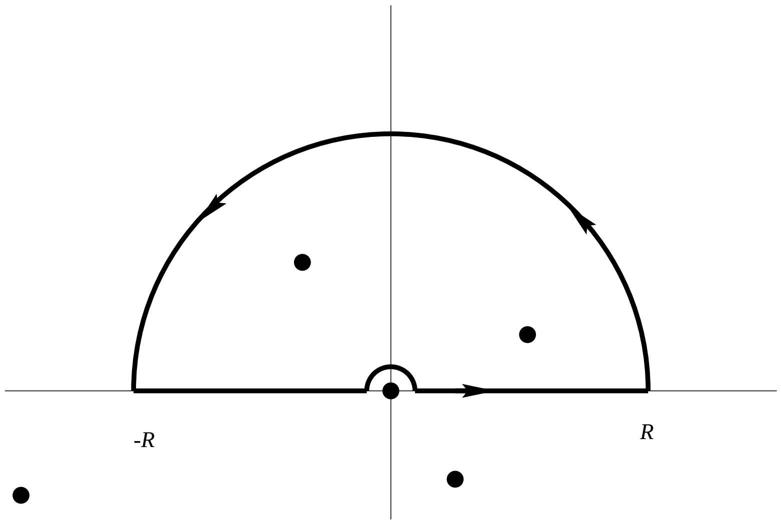

Figure 4: The contour bypasses a pole at the origin

To evaluate the contribution on the semicircular contour γ, we let $z-a = \rho\, e^{\mathrm{i}\,\theta}$, implying that the contour is parameterised (in the direction of the arrow) by taking θ to run from π to 0. Thus near $z = a$ we shall have $f(z) \sim \widetilde{\mathcal{R}}/(z-a)$, where $\widetilde{\mathcal{R}}$ is the residue of the simple pole at $z = a$, and $dz = \mathrm{i}\,\rho\, e^{\mathrm{i}\,\theta}\, d\theta$, whence

$$\int_\gamma f(z)\,dz = \mathrm{i}\,\widetilde{\mathcal{R}} \int_\pi^0 d\theta = -\mathrm{i}\,\pi\,\mathcal{R}\,. \tag{5.234}$$

Sending R to infinity, and ρ to zero, the remaining two terms on the left-hand side of (5.233) define what is called the *Cauchy Principal Value Integral*, denoted by $P\int$,

$$P\int_{-\infty}^{\infty} f(x)\,dx \equiv \int_{-\infty}^{a-\epsilon} f(x)\,dx + \int_{a+\epsilon}^{\infty} f(x)\,dx\,, \tag{5.235}$$

where one takes the limit where the small positive quantity ϵ goes to zero. Such a definition is necessary in order to give meaning to what would otherwise be an ill-defined integral.

In general, we therefore arrive at the result that if $f(z)$ has several simple poles on the real axis, with residues $\widetilde{\mathcal{R}}_k$, as well as poles in the upper half plane with residues $\mathcal{R}_j$, then

$$P\int_{-\infty}^{\infty} f(x)\,dx = 2\pi\,\mathrm{i} \sum_j \mathcal{R}_j + \mathrm{i}\,\pi \sum_k \widetilde{\mathcal{R}}_k\,. \tag{5.236}$$

Here, the principal-value prescription is used to give meaning to the integral, analogously to (5.235), at each of the simple poles on the real axis.

Consider, as an example, $\int_{-\infty}^{\infty} (\sin x)/x\, dx$. Actually, of course, this integrand has no pole on the real axis, since the pole in $1/x$ is cancelled by the zero of $\sin x$. But one way to do the calculation is to say that we shall calculate the imaginary part of

$$\int_{-\infty}^{\infty} \frac{e^{\mathrm{i}\, x}}{x}\, dx = \int_{-\infty}^{\infty} \frac{\cos x}{x}\, dx + \mathrm{i} \int_{-\infty}^{\infty} \frac{\sin x}{x}\, dx\,. \tag{5.237}$$

We must now use the principal-value prescription to give meaning to this integral, since the real part of the integrand in (5.237), namely $(\cos x)/x$, *does* have a pole at $x = 0$. But since we are after the imaginary part, the fact that we have "regulated" the real part of the integral will not upset what we want. Thus from (5.236) we find that

$$P \int_{-\infty}^{\infty} \frac{e^{\mathrm{i}\, x}}{x}\, dx = \mathrm{i}\, \pi\,, \tag{5.238}$$

and so from the imaginary part (which is all there is; the principal-value integral has regulated the ill-defined real part to be zero) we get

$$\int_{-\infty}^{\infty} \frac{\sin x}{x}\, dx = \pi\,. \tag{5.239}$$

Notice that there is another way that we could have handled a pole on the real axis. We could have bypassed aound it the other way, by taking a semicircular contour $\tilde\gamma$ that went into the lower half complex plane instead. Now, the integration (5.234) would be replaced by one where θ ran from $\theta = \pi$ to $\theta = 2\pi$ as one follows in the direction of the arrow, giving, eventually, a contribution $-\mathrm{i}\, \pi\, \widetilde{\mathcal{R}}$ rather than $+\mathrm{i}\, \pi\, \widetilde{\mathcal{R}}$ in (5.236). But all is actually well, because if we make a detour of this kind we should actually now also include the contribution of this pole as an honest pole enclosed by the full contour C, so it will also give a contribution $2\pi\, \mathrm{i}\, \widetilde{\mathcal{R}}$ in the first summation on the right-hand side of (5.236). So at the end of the day, we end up with the same conclusion no matter which way we detour around the pole.

Another common kind of real integral that can be evaluated using the calculus of residues involves the log function. Consider, for example, the following:

$$I \equiv \int_0^{\infty} \frac{\log x\, dx}{(1 + x^2)^2}\,. \tag{5.240}$$

One way to evaluate this is by taking the usual large semicircular contour in the upper half plane, with a little semicircular detour γ (in the upper half plane) bypassing the branch point at $z = 0$, as in Figure 4. We think of running the branch cut of $\log z$ from $z = 0$ to

$z = \infty$, just fractionally *below* the positive real axis. Thus for z on the positive real axis, we shall have simply $\log z = \log x$. If we look just *below* the branch cut, i.e. for $z = x - \mathrm{i}\,\epsilon$, where ϵ is a very small positive constant, we shall have $\log z = \log x + 2\mathrm{i}\,\pi$ in the limit when ϵ goes to zero, since we have effectively swung once around the origin, semding $z \longrightarrow z\, e^{2\mathrm{i}\,\pi}$, to get there.

Then we shall have

$$\int_{-\infty}^{-\rho} \frac{\log x\, dx}{(1+x^2)^2} + \int_\gamma \frac{\log z\, dz}{(1+z^2)^2} + \int_\rho^\infty \frac{\log x\, dx}{(1+x^2)^2} = 2\pi\,\mathrm{i}\,\mathcal{R}\,, \tag{5.241}$$

where $\mathcal{R}$ is the residue of $(\log z)/(1+z^2)^2$ at the double pole at $z = \mathrm{i}$ in the upper half plane. (As usual, we must check that the integrand indeed has the appropriate fall-off property so that the contribution from the large semicircular arc goes to zero; it does.) There are a couple of new features that this example illustrates.

First, consider the integral around the little semicircle γ. Letting $z = \rho\, e^{\mathrm{i}\,\theta}$ there we shall have

$$\int_\gamma \frac{\log z\, dz}{(1+z^2)^2} = -\mathrm{i}\,\rho \int_0^\pi \frac{\log(\rho\, e^{\mathrm{i}\,\theta})\, e^{\mathrm{i}\,\theta}\, d\theta}{(1+\rho^2\, e^{2\mathrm{i}\,\theta})^2}\,. \tag{5.242}$$

This looks alarming at first, but closer inspection reveals that it will give zero, once we take the limit $\rho \longrightarrow 0$. The point is that after writing $\log(\rho\, e^{\mathrm{i}\,\theta}) = \log\rho + \mathrm{i}\,\theta$, we see that the θ integrations will not introduce any divergences, and so the overall factors of ρ or $\rho\,\log\rho$ in the two parts of the answer will both nicely kill off the contributions, as $\rho \longrightarrow 0$.

Next, consider the first integral on the left-hand side of (5.241). For this, we can change variable from x, which takes negative values, to t, say, which is positive. But we need to take care, because of the multi-valuedness of the log function. So we should define

$$x = e^{\mathrm{i}\pi}\, t\,. \tag{5.243}$$

In all places except the log, we can simply interpret this as $x = -t$, but in the log we shall have $\log z = \log(e^{\mathrm{i}\pi}\, t) = \log t + \mathrm{i}\,\pi$. Thus the first integral in (5.241) gives

$$\int_{-\infty}^0 \frac{\log x\, dx}{(1+x^2)^2} = \int_0^\infty \frac{\log t\, dt}{(1+t^2)^2} + \mathrm{i}\,\pi \int_0^\infty \frac{dt}{(1+t^2)^2}\,. \tag{5.244}$$

(Now that we know that there is no contribution from the little semicircle γ, we can just take $\rho = 0$ and forget about it.) The first term on the right-hand side here is of exactly the same form as our original integral I defined in (5.240). The second term on the right is a simple integral. It itself can be done by contour integral methods, as we have seen. Since there is no new subtlety involved in evaluating it, let's just quote the answer, namely

$$\int_0^\infty \frac{dt}{(1+t^2)^2} = \tfrac{1}{4}\pi\,. \tag{5.245}$$

Taking stock, we have now arrived at the result that

$$2I + \tfrac{1}{4}\mathrm{i}\,\pi^2 = 2\pi\,\mathrm{i}\,\mathcal{R}\,. \tag{5.246}$$

It remains only to evaluate the residue of $(\log z)/(1+z^2)^2$ at the double pole at $z = \mathrm{i}$ in the upper half plane. We do this with the standard formula (5.217). Thus we have

$$\mathcal{R} = \frac{d}{dz}\Big[\frac{\log z}{(z+\mathrm{i})^2}\Big]\,, \tag{5.247}$$

to be evaluated at $z = \mathrm{i} = e^{\mathrm{i}\,\pi/2}$. (Note that we should write it explicitly as $e^{\mathrm{i}\,\pi/2}$ in order to know exactly what to do with the $\log z$ term.) Thus we get

$$\mathcal{R} = \tfrac{\mathrm{i}}{4} + \tfrac{1}{8}\pi\,. \tag{5.248}$$

Plugging into (5.246), we see that the imaginary term on the left-hand side is cancelled by the imaginary term in (5.248), leaving just $2I = -\pi/2$. Thus, eventually, we arrive at the result that

$$\int_0^\infty \frac{\log x\, dx}{(1+x^2)^2} = -\tfrac{1}{4}\pi\,. \tag{5.249}$$

Aside from the specifics of this example, there are two main general lessons to be learned from it. The first is that if an integrand has just a logarithmic divergence at some point $z = a$, then the contour integral around a little semicircle or circle centred on $z = a$ will give zero in the limit when its radius ρ goes to zero. This is because the logarithmic divergence of $\log\rho$ is outweighed by the linear factor of ρ coming from writing $dz = \mathrm{i}\,\rho\, e^{\mathrm{i}\,\theta}\, d\theta$.

The second general lesson from this example is that one should pay careful attention to how the a coordinate redefinition is performed, for example when re-expressing an integral along the negative real axis as an integral over a positive variable (like t in our example). In particular, one has to handle the redefinition with appropriate care in the multi-valued log function.

5.8 Summation of Series

Another application of the calculus of residues is for evaluating certain types of infinite series. The idea is the following. We have seen that the functions $\operatorname{cosec}\pi z$ and $\cot\pi z$ have the property of having simple poles at all the integers, whilst otherwise being analytic in the whole finite complex plane. In fact, they are bounded everywhere as one takes $|z|$ to infinity, except along the real axis where the poles lie. Using these functions, we can write down contour integrals that are related to infinite sums.

First, let us note that the residues of the two trigonometric functions are as follows:

- $\pi\,\cot\pi z$ has residue 1 at $z = n$
- $\pi\,\mathrm{cosec}\,\pi z$ has residue $(-1)^n$ at $z = n$

Consider the following integral:

$$I_p \equiv \oint_{C_p} f(z)\,\pi\,\cot\pi z\,, \tag{5.250}$$

where C_p is a closed contour that encloses the poles of $\cot\pi z$ at $z = 0, \pm 1, \pm 2, \ldots, \pm p$, but does not enclose any that lie at any larger value of $|z|$. A typical choice for the contour C_p is a square, centred on the origin, with side $2p+1$, or else a circle, again passing through the points $\pm(p+\frac{1}{2})$. (See Figure 5 below.) Then by the theorem of residues we shall have

$$I_p = 2\pi\,\mathrm{i}\sum_{n=-p}^{p} f(n) + 2\pi\,\mathrm{i}\sum_a \mathcal{R}_a\,, \tag{5.251}$$

where $\mathcal{R}_a$ denotes the residue of $f(z)\,\pi\,\cot\pi z$ at pole number a of the function $f(z)$, and the summation is over all such poles that lie within the contour C_p. In other words, we have simply split the total sum over residues into the first term, which sums over the residues at the known simple poles of $\cot\pi z$, and the second term, which sums over the poles associated with the function $f(z)$ itself. Of course, in the first summation, the residue of $f(z)\,\pi\,\cot\pi z$ at $z = n$ is simply $f(n)$, since the pole in $\pi\,\cot\pi z$ is simple, and itself has residue 1. (We are assuming here that $f(z)$ doesn't itself have poles at the integers.)

Now, it is clear that if we send p to infinity, so that the corresponding contour C_p grows to infinite size and encompasses the whole complex plane, we shall have

$$\oint_{C_\infty} f(z)\,\pi\,\cot\pi z = 2\pi\,\mathrm{i}\sum_{n=-\infty}^{\infty} f(n) + 2\pi\,\mathrm{i}\sum_a \mathcal{R}_a\,, \tag{5.252}$$

where the second sum now ranges over the residues $\mathcal{R}_a$ of $f(z)\,\pi\,\cot\pi z$ at all the poles of $f(z)$. Furthermore, let us suppose that the function $f(z)$ is such that

$$|z\,f(z)| \longrightarrow 0 \quad \text{as} \quad |z| \longrightarrow \infty\,. \tag{5.253}$$

It follows that the integral around the contour C_∞ out at infinity will be zero. Consequently, we obtain the result that

$$\sum_{n=-\infty}^{\infty} f(n) = -\sum_a \mathcal{R}_a\,, \tag{5.254}$$

where the right-hand sum is over the residues $\mathcal{R}_a$ of $f(z)\,\pi\,\cot\pi z$ at all the poles of $f(z)$.

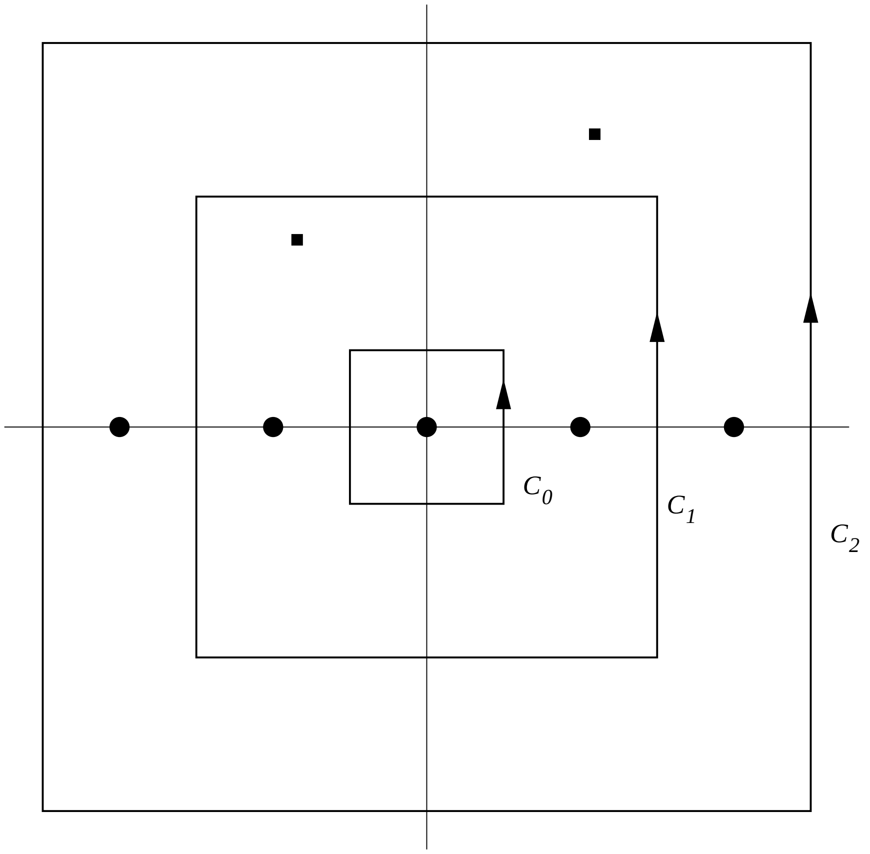

Figure 5: The square contours enclose the poles of $f(z)$ (square dots) and the poles of $\cot\pi z$ or $\operatorname{cosec}\pi z$ (round dots)

In a similar fashion, using $\operatorname{cosec}\pi z$ in place of $\cot\pi z$, we have that

$$\sum_{n=-\infty}^{\infty}(-1)^n\, f(n) = -\sum_a \widetilde{\mathcal{R}}_a\,, \tag{5.255}$$

where the right-hand sum is over the residues of $f(z)\,\pi\operatorname{cosec}\pi z$ at all the poles of $f(z)$.

Consider an example. Suppose we take

$$f(z) = \frac{1}{(z+a)^2}\,. \tag{5.256}$$

This has a double pole at $z=-a$. Using (5.217), we therefore find that the residue of $f(z)\,\pi\ \cot\pi z$ at $z=-a$ is

$$\mathcal{R} = -\pi^2 \operatorname{cosec}^2(\pi a)\,, \tag{5.257}$$

and hence from (5.254) we conclude that

$$\sum_{n=-\infty}^{\infty}\frac{1}{(n+a)^2} = \frac{\pi^2}{\sin^2\pi a}\,. \tag{5.258}$$

We can also evaluate the analgous sum with alternating signs, by using (5.255) instead. Now, we caluate the residue of $(z+a)^{-2}\,\pi\,\mathrm{cosec}\,\pi z$ at the double pole at $z=-a$, and conclude that

$$\sum_{n=-\infty}^{\infty} \frac{(-1)^n}{(n+a)^2} = \frac{\pi^2\,\cos\pi a}{\sin^2\pi a}\,. \tag{5.259}$$

Clearly there are large classes of infinite series that can be summed using these techniques. We shall encounter another example later, in a discussion of the Riemann zeta function.

5.9 Analytic Continuation

Analyticity of a function of a complex variable is a very restrictive condition, and consequently it has many powerful implications. One of these is the concept of *analytic continuation.* Let us begin with an example.

Consider the function $g(z)$, which is *defined* by the power series

$$g(z) \equiv \sum_{n\ge 0} z^n\,. \tag{5.260}$$

It is easily seen, by applying the Cauchy test for convergence, that this series is absolutely convergent for $|z|<1$. It follows, therefore, that the function $g(z)$ defined by (5.260) is analytic inside the unit circle $|z|<1$. It is also true, of course, that $g(z)$ is singular outside the unit circle; the power series diverges.

Of couse (5.260) is a very simple geometric series, and we can see by inspection that it can be summed, when $|z|<1$, to give

$$f(z) = \frac{1}{1-z}\,. \tag{5.261}$$

This is analytic everywhere except for a pole at $z=1$. So we have two functions, $g(z)$ and $f(z)$, which are both analytic inside the unit circle, and indeed they are identical inside the unit circle. However, whereas the function $g(z)$ is singular outside the unit circle, the function $f(z)$ is well-defined and analytic in the entire complex plane, with the exception of the point $z=1$ where it has a simple pole.

It is evident, therefore, that we can view $f(z)=1/(1-z)$ as an extrapolation, or continuation, of the function $g(z)=1+z+z^2+\cdots$ outside its circle of convergence. As we shall prove below, there is an enormously powerful statement that can be made; the function $1/(1-z)$ is the *unique* analyic continuation of the original function $g(z)$ defined in the unit circle by (5.260). This uniqueness is absolutely crucial, since it means that one can sensibly talk about *the* analytic continuation of a function that is initially defined in some restricted region of the complex plane. *A priori*, one might have imagined that there could be any number of ways of defining functions that coincided with $g(z)$ inside the unit circle, but that extrapolated in all sorts of different ways as one went outside the unit circle. And indeed, if we don't place the extra, and very powerful, restriction of *analyticity*, then that would be exactly the case. We could indeed dream up all sorts of non-analytic functions that agreed with $g(z)$ inside the unit circle, and that extrapolated in arbitrary ways outside the unit circle.[23] The amazing thing is that if we insist that the extrapolating function be analytic, then there is precisely one, and only one, analytic continuation.

In the present example, we have the luxury of knowing that the function $g(z)$, *defined* by the series expansion (5.260), actually sums to give $1/(1-z)$ for any z within the unit circle. This immediately allows us to deduce, in this example, that the analytic continuation of $g(z)$ is precisely given by

$$g(z) = \frac{1}{1-z}\,, \tag{5.262}$$

which is defined everywhere in the complex plane except at $z = 1$. So in this toy example, we know what the function "really is."

Suppose, for a moment, that we didn't know that the series (5.260) could be summed to give (5.262). We could, however, discover that $g(z)$ defined by (5.260) gave perfectly sensible results for any z within the unit circle. (For example, by applying the Cauchy test for absolute convergence of the series.) Suppose that we use these results to evaluate $f(z)$ in the neighbourhood of the point $z = -\frac{1}{2}$. This allows us, by using Taylor's theorem, to construct a series expansion for $g(z)$ around the point $z = -\frac{1}{2}$:

$$g(z) = \sum_{n\ge 0} \frac{g^{(n)}(-\frac{1}{2})}{n!}\,(z+\tfrac{1}{2})^n\,. \tag{5.263}$$

Where does this converge? We know from the earlier general discussion that it will converge within a circle of radius R centred on $z = -\frac{1}{2}$, where R is the distance from $z = -\frac{1}{2}$ to the nearest singularity. We know that actually, this singularity is at $z = 1$. Therefore our new Taylor expansion (5.263) is convergent in a circle of radius $\frac{3}{2}$, centered on $z = -\frac{1}{2}$. This circle of convergence, and the original one, are depicted in Figure 6 below. We see that this process has taken us outside the original unit circle; we are now able to evaluate "the

[23] We could, for example, simply *define* a function $F(z)$ such that $F(z) \equiv g(z)$ for $|z| < 1$, and $F(z) \equiv h(z)$ for $|z| \ge 1$, where $h(z)$ is *any function we wish*. But the function will in general be horribly non-analytic on the unit circle $|z| = 1$ where the changeover occurs.

function $g(z)$" in a region outside the unit circle, where its original power-series expansion (5.260) does not converge.[24]

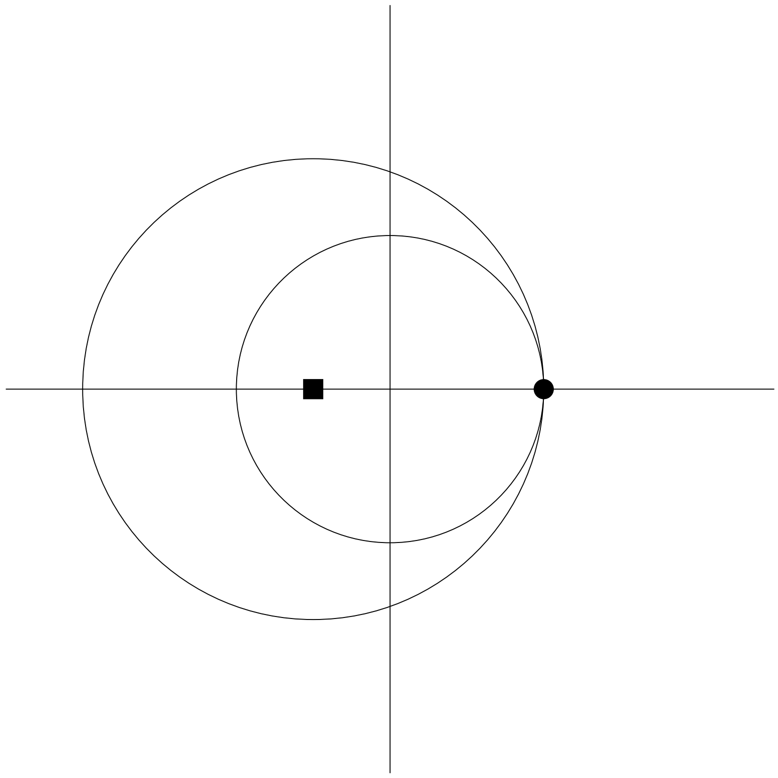

Figure 6: The circles of convergence for the two series

It should be clear that be repeated use of this technique, we can eventually cover the entire complex plane, and hence construct the analytic continuation of $g(z)$ from its original definition (5.260) to a function defined everywhere except at $z = 1$.

The crucial point here is that the process of analytic continuation is a unique one. To show this, we can establish the following theorem:

Let $f(z)$ and $g(z)$ be two functions that are analytic in a region D, and suppose that they are equal on an infinite set of points having a limit point z_0 in D. Then $f(z) \equiv g(z)$ for all points z in D.

[24]Secretly, we know that the power series we will just have obtained is nothing but the standard Taylor expansion of $1/(1-z)$ around the point $z = -\frac{1}{2}$:

$$\frac{1}{1-z} = \tfrac{2}{3} + \tfrac{4}{9}(z+\tfrac{1}{2}) + \tfrac{8}{27}(z+\tfrac{1}{2})^2 + \tfrac{16}{81}(z+\tfrac{1}{2})^3 + \cdots , \tag{5.264}$$

which indeed converges in a circle of radius $\frac{3}{2}$.

In other words, if we know that the two analytic functions $f(z)$ and $g(z)$ agree on an arc of points ending at point[25] z_0 in D, then they must agree everywhere in D. (Note that we do not even need to know that they agree on a smooth arc; it is sufficient even to know that they agree on a discrete set of points that get denser and denser until the end of the arc at $z = z_0$ is reached.)

To prove this theorem, we first define $h(z) = f(z) - g(z)$. Thus we know that $h(z)$ is analytic in D, and it vanishes on an infinite set of points with limit point z_0. We are required to prove that $h(z)$ must be zero everywhere in D. We do this by expanding $h(z)$ in a Taylor series around $z = z_0$:

$$h(z) = \sum_{k=0}^{\infty} a_k \, (z - z_0)^k = a_0 + a_1 \, (z - z_0) + \cdots \,, \tag{5.265}$$

which converges in some neighbourhood of z_0 since $h(z)$ is analytic in the neighbourhood of $z = z_0$. Since we want to prove that $h(z) = 0$, this means that we want to show that all the coefficients a_k are zero.

Of course since $h(z_0) = 0$ we know at least that $a_0 = 0$. We shall prove that all the a_k are zero by the time-honoured procedure of supposing that this is not true, and then arriving at a contradiction. Let us suppose that a_m, for some m, is the first non-zero a_k coefficient. This means that if we define

$$\begin{aligned} p(z) \quad &\equiv \quad (z - z_0)^{-m} \, h(z) = (z - z_0)^{-m} \, \sum_{k=m}^{\infty} a_k \, (z - z_0)^k \,, \\ &= \quad a_m + a_{m+1} \, (z - z_0) + \cdots \,, \end{aligned} \tag{5.266}$$

then $p(z)$ is an analytic function, and its Taylor series is therefore also convergent, in the neighbourhood of $z = z_0$. Now comes the punch-line. We know that $h(z)$ is zero for all the points $z = z_n$ in that infinite set that has z_0 as a limit point. Thus in particular there are points z_n with n very large that are arbitrarily close to $z = z_0$, and at which $h(z)$ vanishes. It follows from its definition that $p(z)$ must also vanish at these points. But since the Taylor series for $p(z)$ is convergent for points z near to $z = z_0$, it follows that for $p(z_n)$ to vanish when n is very large we must have $a_m = 0$, since all the higher terms in the Taylor series would be negligible. But this contradicts our assumption that a_m was the first non-vanishing coefficient in (5.265). Thus the premise that there exists a first non-vanishing coefficient was false, and so it must be that *all* the coefficients a_k vanish. This proves that $h(z) = 0$, which is what we wanted to show.

[25] An example of such a set of points would be $z_n = z_0 + 1/n$, with $n = 1, 2, 3 \ldots$.

The above proof shows that $h(z)$ must vanish within the circle of convergence, centered on $z = z_0$, of the Taylor series (5.265). By repeating the discussion as necessary, we can extend this region gradually until the whole of the domain D has been covered. Thus we have established that $f(z) = g(z)$ everywhere in D, if they agree on an infinite set of points with limit point z_0.

By this means, we may eventually seek to analytically extend the function to the whole complex plane. There may well be singularities at certain places, but provided we don't run into a solid "wall" of singularities, we can get around them and extend the definition of the function as far as we wish. Of course if the function has branch points, then we will encounter all the usual multi-valuedness issues as we seek to extend the function.

Let us go back for a moment to our example with the function $g(z)$ that was originally defined by the power series (5.260). We can now immediately invoke this theorem. It is easily established that the series (5.260) sums to give $1/(1-z)$ within the unit circle. Thus we have two analytic functions, namely $g(z)$ defined by (5.260) and $f(z)$ defined by (5.261) that agree in the entire unit circle. (Much more than just an arc with a limit point, in fact!) Therefore, it follows that there is a unique way to extend analytically outside the unit circle. Since $f(z) = 1/(1-z)$ is certainly analytic outside the unit circle, it follows that the function $1/(1-z)$ is the unique analytic extension of $g(z)$ defined by the power series (5.260).

Let us now consider a less trivial example, to show the power of analytic continuation.

5.10 The Gamma Function

The Gamma function $\Gamma(z)$ can be represented by the integral

$$\Gamma(z) = \int_0^\infty e^{-t}\, t^{z-1}\, dt\,, \tag{5.267}$$

which converges if $\mathrm{Re}(z) > 0$. It is easy to see that if $\mathrm{Re}(z) > 1$ then we can perform an integration by parts to obtain

$$\Gamma(z) = (z-1) \int_0^\infty e^{-t}\, t^{z-2}\, dt - \Big[e^{-t}\, t^{z-1}\Big]_0^\infty = (z-1)\, \Gamma(z-1)\,, \tag{5.268}$$

since the boundary term then gives no contribution. Shifting by 1 for convenience, we have

$$\Gamma(z+1) = z\, \Gamma(z)\,. \tag{5.269}$$

One easily sees that if z is a positive integer k, the solution to this recursion relation is $\Gamma(k) = (k-1)!$, since it is easily established by elementary integration that $\Gamma(1) = 1$. The responsibility for the rather tiresome shift by 1 in the relation $\Gamma(k) = (k-1)!$ lies with Leonhard Euler.

Of course the definition (5.267) is valid only when the integral converges. It's clear that the e^{-t} factor ensures that there is no trouble from the upper limit of integration, but from $t = 0$ there will be a divergence unless $\text{Re}(z) > 0$. Furthermore, for $\text{Re}(z) > 0$ it is clear that we can differentiate (5.267) with respect to z as many times as we wish, and the integrals will still converge.[26] Thus $\Gamma(z)$ defined by (5.267) is *finite* and analytic for all points with $\text{Re}(z) > 0$.

We can now use (5.269) in order to give an analytic contiuation of $\Gamma(z)$ into the region where $\text{Re}(z) \le 0$. Specifically, if we write (5.269) as

$$\Gamma(z) = \frac{\Gamma(z+1)}{z}\,, \tag{5.271}$$

then this gives a way of evaluating $\Gamma(z)$ for points in the strip $-1+\epsilon < \text{Re}(z) < \epsilon$ (ϵ a small positive quantity) in terms of $\Gamma(z+1)$ at points with $\text{Re}(z+1) > 0$, where $\Gamma(z+1)$ is known to be analytic. The function so defined, and the original Gamma function, have an overlapping region of convergence, and so we can make an analytic continuation into the strip $-1+\epsilon < \text{Re}(z) < \epsilon$. The process can then be applied iteratively, to cover more and more strips over to the left-hand side of the complex plane, until the whole plane has been covered by the analytic extension. Thus by sending $z \to z+1$ in (5.271) we may write

$$\Gamma(z+1) = \frac{\Gamma(z+2)}{z+1}\,, \tag{5.272}$$

and plugging this into (5.271) itself we get

$$\Gamma(z) = \frac{\Gamma(z+2)}{(z+1)\,z}\,. \tag{5.273}$$

The right-hand side is analytic for $\text{Re}(z) > -2$, save for the two manifest poles at $z = 0$ and $z = -1$, and so this has provided us with an analytic continuation of $\Gamma(z)$ into the region $\text{Re}(z) > -2$. In the next iteration we use (5.271) with $z \to z+2$ to express $\Gamma(z+2)$ as $\Gamma(z+3)/(z+2)$, hence giving

$$\Gamma(z) = \frac{\Gamma(z+3)}{(z+2)(z+1)\,z}\,, \tag{5.274}$$

[26] Write $t^z = e^{z\,\log t}$, and so, for example,

$$\Gamma'(z) = \int_0^\infty dt\, t^{z-1}\, \log t\, e^{-t}\,. \tag{5.270}$$

Now matter how many powers of $\log t$ are brought down by repeated differentiation, the factor of t^{z-1} will ensure convergence at $t = 0$.

valid for $\mathrm{Re}(z) > -3$, and so on.

Of course the analytically continued function $\Gamma(z)$ is not necessarily analytic at every point in the complex plane, and indeed, we are already seeing, it has isolated poles. To explore the behaviour of $\Gamma(z)$ in the region of some point z with $\mathrm{Re}(z) \le 0$, we first iterate (5.269) just as many times n as are necessary in order to express $\Gamma(z)$ in terms of $\Gamma(z+n+1)$:

$$\Gamma(z) = \frac{\Gamma(z+n+1)}{(z+n)(z+n-1)(z+n-2)\cdots z}\,, \tag{5.275}$$

where we choose n so that $\mathrm{Re}(z+n+1) > 0$ but $\mathrm{Re}(z+n) < 0$. Since we have already established that $\Gamma(z+n+1)$ will therefore be finite, it follows that the only singularities of $\Gamma(z)$ can come from places where the denominator in (5.275) vanishes. This will therefore happen when $z = 0$ or z is a negative integer.

To study the precise behaviour near the point $z = -n$, we may set $z = -n + \epsilon$, where $|\epsilon| << 1$, and use (5.275) to give

$$\Gamma(-n+\epsilon) = \frac{(-1)^n\,\Gamma(1+\epsilon)}{(n-\epsilon)(n-\epsilon-1)\cdots(1-\epsilon)\,\epsilon} = \frac{(-1)^n}{n\,(n-1)\cdots 2\cdot 1\,\epsilon} + \cdots\,, \tag{5.276}$$

where the terms represented by $\cdots$ are analytic in ϵ. Thus there is a simple pole at $\epsilon = 0$. Its residue is calulated by multiplying (5.276) by ϵ and taking the limit $\epsilon \longrightarrow 0$. Thus we conclude that $\Gamma(z)$ is meromorphic in the whole finite complex plane, with simple poles at the points $z = 0,\ -1,\ -2,\ -3, \ldots$, with the residue at $z = -n$ being $(-1)^n/n!$. (Since $\Gamma(1) = 1$.)

The regular spacing of the poles of $\Gamma(z)$ is reminiscent of the poles of the functions $\mathrm{cosec}\,\pi z$ or $\cot\pi z$. Of course in these cases, they have simple poles at *all* the integers; zero negative and positive. We can in fact make a function with precisely this property out of $\Gamma(z)$, by writing the product

$$\Gamma(z)\,\Gamma(1-z)\,. \tag{5.277}$$

From what we saw above, it is clear that this function will have simple poles at precisely all the integers. Might it be that this function is related to $\mathrm{cosec}\,\pi z$ or $\cot\pi z$?

To answer this, consider again the original integral representation (5.267) for $\Gamma(z)$, and now make the change of variables $t \longrightarrow t^2$. This implies $dt/t \longrightarrow 2dt/t$, and so we shall have

$$\Gamma(z) = 2\int_0^\infty e^{-t^2}\, t^{2z-1}\, dt\,. \tag{5.278}$$

Thus we may write

$$\Gamma(a)\,\Gamma(1-a) = 4\int_0^\infty dx \int_0^\infty dy\, e^{-(x^2+y^2)}\, x^{2a-1}\, y^{-2a+1}\,. \tag{5.279}$$

Introducing polar coordinates *via* $x = r\,\cos\theta$, $y = r\,\sin\theta$, we therefore get

$$\Gamma(a)\,\Gamma(1-a) = 4\int_0^{\frac{1}{2}\pi} (\cot\theta)^{2a-1}\,d\theta \int_0^\infty r\,e^{-r^2}\,dr\,. \tag{5.280}$$

The r integration is trivially performed, giving a factor of $\frac{1}{2}$, and so we have

$$\Gamma(a)\,\Gamma(1-a) = 2\int_0^{\frac{1}{2}\pi} (\cot\theta)^{2a-1}\,d\theta\,. \tag{5.281}$$

Now, we let $s = \cot\theta$. This gives

$$\Gamma(a)\,\Gamma(1-a) = 2\int_0^\infty \frac{s^{2a-1}\,ds}{1+s^2}\,. \tag{5.282}$$

If we restrict a such that $0 < \text{Re}(a) < 1$, this integral falls into the category of type 3 that we discussed a couple of sections ago. Thus we have

$$\Gamma(a)\,\Gamma(1-a) = \frac{2\pi}{\sin(2\pi\,a)} \sum_c \mathcal{R}_c\,, \tag{5.283}$$

where $\mathcal{R}_c$ are the residues at the poles of $(-z)^{2a-1}/(1+z^2)$. These poles lie at $z = \pm\text{i}$, and the residues are easily seen to be $\frac{1}{2}e^{\pm\text{i}\,\pi\,a}$. Thus we get

$$\begin{aligned} \Gamma(a)\,\Gamma(1-a) &= \frac{2\pi}{\sin(2\pi\,a)}\,\cos(\pi\,a) = \frac{2\pi\,\cos(\pi\,a)}{2\sin(\pi\,a)\,\cos(\pi\,a)}\,, \\ &= \frac{\pi}{\sin\pi\,a}\,. \end{aligned} \tag{5.284}$$

Although we derived this by restricting a such that $0 < \text{Re}(a) < 1$ in order to ensure convergence in the integration, we can use the now-familiar technique of analytic continuation and conclude that

$$\Gamma(z)\,\Gamma(1-z) = \frac{\pi}{\sin\pi\,z}\,, \tag{5.285}$$

in the whole complex plane. This result, known as the reflection formula, is one that will be useful in the next section, when we shall discuss the Riemann Zeta function.

Before moving on to the Riemann Zeta function, let us first use (5.285) to uncover a couple more properties of the Gamma function. The first of these is a simple fact, namely that

$$\Gamma(\tfrac{1}{2}) = \sqrt{\pi}\,. \tag{5.286}$$

We see this by setting $z = \frac{1}{2}$ in (5.285).

The second, more significant, property of $\Gamma(z)$ that we can deduce from (5.285) is that $\Gamma(z)^{-1}$ an *entire* function. That is to say, $\Gamma(z)^{-1}$ is analytic everywhere in the finite complex plane. Since we have already seen that the only singularities of $\Gamma(z)$ are poles, this means that we need only show that $\Gamma(z)$ has no zeros in the finite complex plane. Looking at (5.285) we see that if it were to be the case that $\Gamma(z) = 0$ for some value of z, then it would have to be that $\Gamma(1-z)$ were infinite there.[27] But we know precisely where $\Gamma(1-z)$ is infinite, namely the poles at $z = 1, 2, 3\ldots$, and $\Gamma(z)$ is certainly not zero there.[28] Therefore $\Gamma(z)$ is everywhere non-zero in the finite complex plane. Consequently, $\Gamma(z)^{-1}$ is analytic everywhere in the finite complex plane, thus proving the contention that $\Gamma(z)^{-1}$ is an entire function.

Before closing this section, we may observe that we can also give a contour integral representation for the Gamma function. This will have the nice feature that it will provide us directly with an expression for $\Gamma(z)$ that is valid in the whole complex plane. Consider first the *Hankel integral*

$$\Gamma(z) = -\frac{1}{2\,\mathrm{i}\,\sin\pi z}\int_C e^{-t}\,(-t)^{z-1}\,dt\,, \tag{5.287}$$

where we integrate in the complex t-plane around the so-called *Hankel Contour* depicted in Figure 7 below. This starts at $+\infty$ just above the real axis, swings around the origin, and goes out to $+\infty$ again just below the real axis. As usual, we shall run the branch cut for the multi-valued function $(-t)^{z-1}$ along the positive real axis in the complex t plane.

We see can deform the contour in Figure 7 into the contour depicted in Figure 8, since no singularities are crossed in the process. If $\mathrm{Re}(z) > 0$, there will be no contribution from integrating around the small circle surrounding the origin, in the limit where its radius is sent to zero. Hence the contour integral is re-expressible simply in terms of the two semi-infinite line integrals just above and below the real axis.

The integrals along the lower and upper causeways in Figure 8, we follow the same procedure that we have used before. We define the phase of $(-t)^z$ to be zero when t lies on the negative real t axis, and run the branch cut along the positive real t axis. For the integral below the real axis, we therefore have $(-t) = e^{\pi\,\mathrm{i}}\,x$, with x running from 0 to $+\infty$. For the integral above the real axis, we have $(-t) = e^{-\mathrm{i}\,\pi}\,x$, with x running from $+\infty$ to 0. Consequently, we get

$$\begin{aligned}\int_C e^{-t}\,(-t)^{z-1}\,dz &= (e^{\mathrm{i}\,\pi\,(z-1)} - e^{-\mathrm{i}\,\pi\,(z-1)})\int_0^\infty e^{-t}\,t^{z-1}\,dt\,,\\ &= -2\,\mathrm{i}\,\sin(\pi z)\int_0^\infty e^{-t}\,t^{z-1}\,dt\,,\end{aligned} \tag{5.288}$$

[27]Recall that $\sin\pi z$ is an entire function, and it therefore has no singularity in the finite complex plane. Consequently, $1/(\sin\pi z)$ must be non-vanishing for all finite z.

[28]Instead, the poles of $\Gamma(1-z)$ at $z = 1, 2, 3\ldots$ are balanced in (5.285) by the poles in $1/\sin(\pi\,z)$.

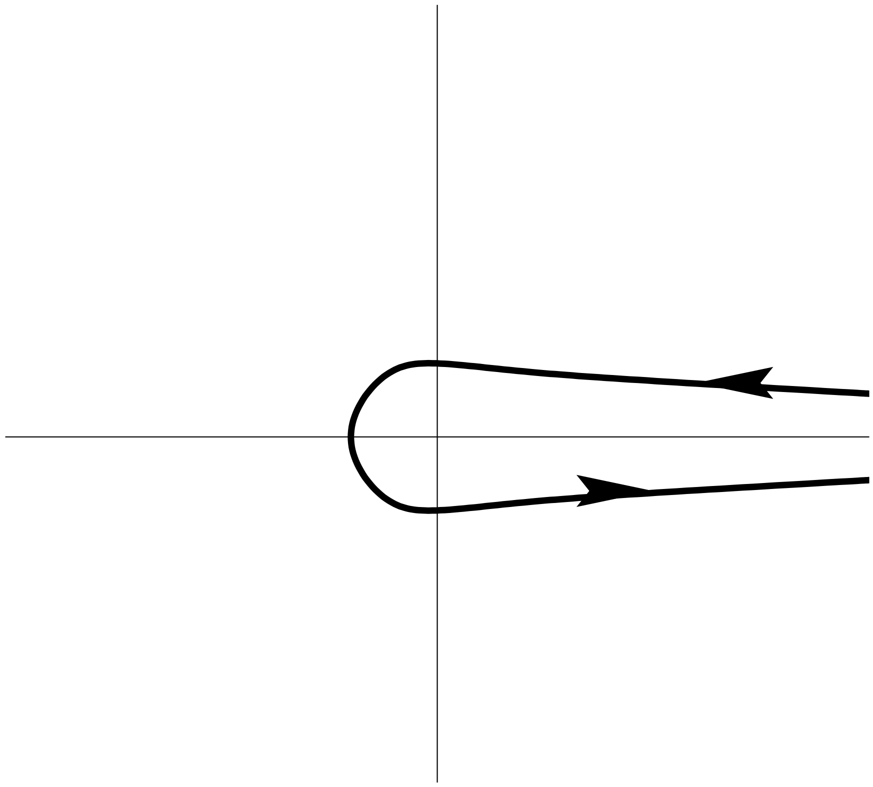

Figure 7: The Hankel contour

and hence we see that (5.287) has reduced to the original real integral expression (5.267) when $\mathrm{Re}(z) > 0$. However, the integral in the expression (5.287) has a much wider applicability; it is actually single-valued and analytic for *all* z. (Recall that we are integrating around the Hankel contour, which does not pass through the point $t = 0$, and so there is no reason for any singularity to arise, for any value of z.) The poles in $\Gamma(z)$ (which we know from our earlier discussion to occur at $z = 0, -1, -2, \ldots$) must therefore be due entirely to the $1/\sin(\pi z)$ prefactor in (5.288. Indeed, as we saw a while ago, $1/\sin(\pi z)$ has simple poles when z is an integer.[29]

Combining (5.287) with (5.285), we can give another contour integral expression for $\Gamma(z)$, namely

$$\frac{1}{\Gamma(z)} = -\frac{1}{2\pi\,\mathrm{i}} \int_C e^{-t}\,(-t)^{-z}\,dt\,, \tag{5.289}$$

[29]The reason why (5.288) doesn't also imply that $\Gamma(z)$ has simple poles when z is a positive integer is that the integral itself vanishes when z is a positive integer, and this cancels out the pole from $1/\sin(\pi z)$. This vanishing can be seen from the fact that when z is a positive integer, the integrand is analytic (there is no longer a branch cut), the contour can be closed off at infinity to make a closed contour encircling the origin, and hence Cauchy's theorem implies the integral vanishes.

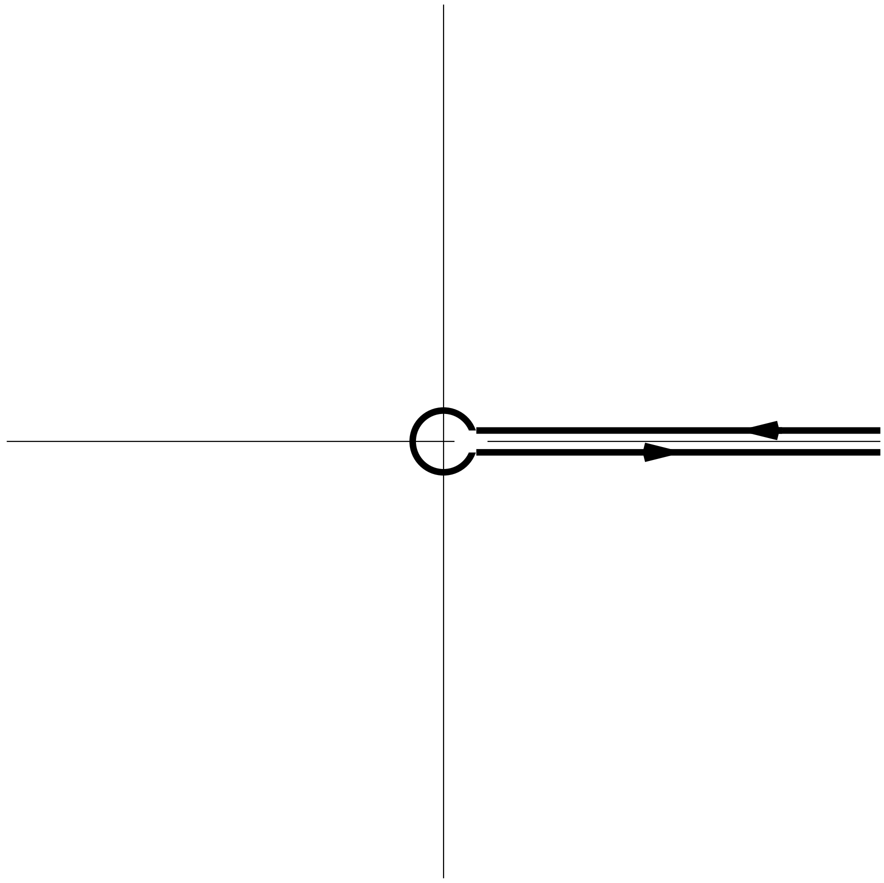

Figure 8: The deformation of the Hankel contour

where we again integrate around the Hankel contour of Figure 7, in the complex t plane. Again, this integral is valid for all z. Indeed with this expression we see again the result that we previously deduced from (5.285), that $\Gamma(z)^{-1}$ is an *entire* function, having no singularities anywhere in the finite complex plane.

A pause for reflection is appropriate here. What we have shown is that $\Gamma(z)$ defined by (5.287) or (5.289) gives the analytic continuation of our original Gamma function (5.267) to the entire complex plane, where it is analytic except for simple poles at $z = 0, -1, -2, \ldots$. How is it that these contour integrals do better than the previous real integral (5.267), which only converged when $\text{Re}(z) > 0$? The crucial point is that in our derivation, when we related the real integral in (5.267) to the contour integral (5.287), we noted that the contribution from the little circle as the contour swung around the origin would go to zero provided that the real part of z was greater than 0.

So what has happened is that we have re-expressed the real integral in (5.267) in terms of a contour integral of the form (5.287), which gives the same answer when the real part of z is greater than 0, but it disagrees when the real part of z is ≤ 0? In fact it disagrees by the having the rather nice feature of being convergent and analytic when $\text{Re}(z) \le 0$, unlike the real integral that diverges. So as we wander off westwards in the complex z plane we wave a fond farewell to the real integral, with its divergent result, and adopt instead the result from the contour integral, which happily provides us with analytic answers even when $\text{Re}(z) \le 0$. We should not be worried by the fact that the integrals are disagreeing there; quite the contrary, in fact. The whole point of the exercise was to find a better way of representing the function, to cover a wider region in the complex plane. If we had merely reproduced the bad behaviour of the original integral in (5.267), we would have achieved nothing by introducing the contour integrals (5.287) and (5.289).

Now we turn to the Riemman Zeta function, as a slightly more intricate example of the analytic continuation of a function of a complex variable.

5.11 The Riemann Zeta Function

Consider the *Riemman Zeta Function*, $\zeta(s)$. This is originally defined by

$$\zeta(s) \equiv \sum_{n=1}^{\infty} \frac{1}{n^s}\,. \tag{5.290}$$

This sum converges whenever the real part of s is greater than 1. (For example, $\zeta(2) = \sum_{n\ge 1} n^{-2}$ can be shown to equal $\pi^2/6$, whereas $\zeta(1) = \sum_{n\ge 1} n^{-1}$ is logarithmically divergent. The sum is more and more divergent as $\text{Re}(s)$ becomes less than 1.)

Since the series (5.290) defining $\zeta(s)$ is convergent everywhere to the right of the line $\text{Re}(s) = 1$ in the complex plane, it follows that $\zeta(s)$ is analytic in that region. It is reasonable to ask what is its analytic continuation over to the left of $\text{Re}(s) = 1$. As we have already seen from the simple example of $f(z) = 1/(1-z)$, the mere fact that our original power series diverges in the region with $\text{Re}(s) \le 0$ does not in any way imply that the "actual" function $\zeta(s)$ will behave badly there. It is just our power series that is inadequate.

How do we do better? To begin, recall that we define the Gamma function $\Gamma(s)$ by

$$\Gamma(s) = \int_0^\infty e^{-u}\, u^{s-1}\, du \tag{5.291}$$

We saw in the previous section that if $s = k$, where k is an integer, then $\Gamma(k)$ is nothing but the factorial function $(k-1)!$. If we now let $u = n\,t$, then we see that

$$\Gamma(s) = n^s \int_0^\infty e^{-n\,t}\, t^{s-1}\, dt\,. \tag{5.292}$$

We can turn this around, to get an expression for n^{-s}.

Plugging into the definition (5.290) of the zeta function, we therefore have

$$\zeta(s) = \frac{1}{\Gamma(s)} \sum_{n=1}^{\infty} \int_0^\infty e^{-n\,t}\, t^{s-1}\, dt\,. \tag{5.293}$$

Taking the summation through the integral, we see that we have a simple geometric series, which can be summed explicitly:

$$\sum_{n=1}^{\infty} e^{-n\,t} = \frac{1}{1-e^{-t}} - 1 = \frac{1}{e^t - 1}\,, \tag{5.294}$$

and hence we arrive at the following integral representation for the zeta function:

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1}\, dt}{e^t - 1}\,. \tag{5.295}$$

So far so good, but actually we haven't yet managed to cross the barrier of the $\mathrm{Re}(s) = 1$ line in the complex plane. The denominator in the integrand goes to zero like t as t tends to zero, so to avoid a divergence from the integration at the lower limit $t = 0$, we must insist that the real part of s should be greater than 1. This is the same restriction that we encountered for the original power series (5.290). What we do now is to turn our real integral (5.295) into a complex contour integral, using the same sort of ideas that we used in the previous section.

To do this, consider the integral

$$\int_C \frac{(-z)^{s-1}\, dz}{e^z - 1}\,, \tag{5.296}$$

where C is the same Hankel contour, depicted in Figure 7, that we used in the discussion of the Gamma function in the previous section. Since the integrand we are considering here clearly has poles at $z = 2\pi\,\mathrm{i}\,n$ for all the integers n, we must make sure that as it circles round the origin, the Hankel contour keeps close enough to the origin (with passing through it) so that it does not encompass any of the poles at $z = \pm 2\pi\,\mathrm{i}, \pm 4\pi\,\mathrm{i}, \ldots$.

By methods analogous to those we used previously, we see that we can again deform this into the contour depicted in Figure 8, where the small circle around the origin will be sent to zero radius. It is clear that there is no contribution from the little circle, provided that the real part of s is greater than 1. Hence the contour integral is re-expressible simply in terms of the two semi-infinite line integrals just above and below the real axis.

As usual, we choose to run the branch cut of the function $(-z)^{s-1}$ along the positive real axis. For the integral below the real axis, we shall then have $(-z) = e^{\pi\,\mathrm{i}}\, t$, with t running from 0 to $+\infty$. For the integral above the real axis, we shall have $(-z) = e^{-\mathrm{i}\,\pi}\, t$, with t running from $+\infty$ to 0. Consequently, we get

$$\int_C \frac{(-z)^{s-1}\, dz}{e^z - 1} = \Big(e^{\mathrm{i}\,\pi\,(s-1)} - e^{-\mathrm{i}\,\pi\,(s-1)}\Big) \int_0^\infty \frac{t^{s-1}\, dt}{e^t - 1} = -2\mathrm{i}\, \sin \pi s \int_0^\infty \frac{t^{s-1}\, dt}{e^t - 1}\,, \tag{5.297}$$

From (5.295), this means that we have a new expression for the zeta function, as

$$\zeta(s) = -\frac{1}{2\mathrm{i}\,\Gamma(s)\,\sin\pi s}\int_C \frac{(-z)^{s-1}\,dz}{e^z-1}\,. \tag{5.298}$$

We can neaten this result up a bit more, if we make use of the reflection formula (5.285) satisfied by the Gamma function, which we proved in the previous section:

$$\Gamma(s)\,\Gamma(1-s) = \frac{\pi}{\sin\pi s}\,. \tag{5.299}$$

Using this in (5.298), we arrive at the final result

$$\zeta(s) = -\frac{\Gamma(1-s)}{2\pi\,\mathrm{i}}\int_C \frac{(-z)^{s-1}\,dz}{e^z-1}\,. \tag{5.300}$$

Now comes the punch-line. The integral in (5.300) is a single-valued and analytic function of s *for all values of* s. (Recall that it is evaluated using the Hankel contour in Figure 7, which does not pass through $z=0$. And far out at the right-hand side of the Hankel contour, the e^z factor in the denominator will ensure rapid convergence. Thus there is no reason for any singular behaviour.) Consequently, the only possible non-analyticity of the zeta function can come from the $\Gamma(1-s)$ prefactor. Now, we studied the singularities of the Gamma function in the previous section. The answer is that $\Gamma(1-s)$ has simple poles at $s=1,2,3,\ldots$, and no other singularities. So these are the only possible points in the finite complex plane where $\zeta(s)$ might have poles. But we already know that $\zeta(s)$ is analytic whenever the real part of s is greater than 1. So it must in fact be the case that the poles of $\Gamma(1-s)$ at $s=2,3,\ldots$ are exactly cancelled by zeros coming from the integral in (5.300). Only the pole at $s=1$ might survive, since we have no independent argument that tells us that $\zeta(s)$ is analytic there. And in fact there *is* a pole in $\zeta(s)$ there.

To see this, we need only to evaluate the integral in (5.300) at $s=1$. This is an easy task. It is given by

$$\frac{1}{2\pi\,\mathrm{i}}\int_C \frac{dz}{e^z-1}\,. \tag{5.301}$$

Now, since we no longer have a multi-valued function in the integrand we don't have to worry about a branch cut along the positive real axis. The integrand has become infinitesimally small out at the right-hand ends of the Hankel contour, and so we can simply join the two ends together without affecting the value of the integral. We now have a closed contour encircling the origin, and so we can evaluate it using the residue theorem; we just need to know the residue of the integrand at $z=0$. Doing the series expansion, one finds

$$\frac{1}{e^z-1} = \frac{1}{z} - \tfrac{1}{2} + \tfrac{1}{12}z - \tfrac{1}{720}\,z^3 + \cdots \tag{5.302}$$

so the residue is 1. From (5.300), this means that near to $s = 1$ we shall have

$$\zeta(s) \sim -\Gamma(1-s)\,. \tag{5.303}$$

In fact $\Gamma(1-s)$ has a simple pole of residue -1 at $s = 1$, as we saw in the previous section, and so the upshot is that $\zeta(s)$ has a simple pole of residue $+1$ at $s = 1$, but it is otherwise analytic everywhere.

It is interesting to try working out $\zeta(s)$ for some values of s that were inaccessible in the original series definition (5.290). For example, let us consider $\zeta(0)$. From (5.300) we therefore have

$$\zeta(0) = \frac{1}{2\pi\,\mathrm{i}} \int_C \frac{dz}{z\,(e^z - 1)}\,, \tag{5.304}$$

where we have used that $\Gamma(1) = 1$. Again, we can close off the Hankel contour of Figure 7 out near $+\infty$, since there is no branch cut, and the e^z in the denominator means that the integrand is vanishly small there. We therefore just need to use the calculus of residues to evaluate (5.304), for a closed contour encircling the second-order pole at $z = 0$. For this, we have

$$\frac{1}{z\,(e^z - 1)} = \frac{1}{z^2} - \frac{1}{2z} + \frac{1}{12} + \cdots\,, \tag{5.305}$$

showing that the residue is $-\frac{1}{2}$. Thus we obtain the result

$$\zeta(0) = -\tfrac{1}{2}\,. \tag{5.306}$$

One can view this result rather whimsically as a "regularisation" of the divergent expression that one would obtain from the original series definition of $\zeta(s)$ in (5.290):

$$\zeta(0) = \sum_{n\ge 1} n^0 = \sum_{n\ge 1} 1 = 1 + 1 + 1 + 1 + \cdots = -\tfrac{1}{2}\,. \tag{5.307}$$

Actually, this strange-looking formula is not entirely whimsical. It is precisely the sort of divergent sum that arises in a typical Feynman diagram loop calculation in quantum field theory (corresponding, for example, to summing the zero-point energies of an infinite number of harmonic oscillators). The whole subtlety of handling the infinities in quantum field theory is concerned with how to recognise and subtract out unphysical divergences associated, for example, with the infinite zero-point energy of the vacuum. This process of renormalisation and regularisation can actually, remarkably, be made respectable, and in particular, it can be shown that the final results are independent of the regularisation scheme that one uses. One scheme that has been developed is known as "Zeta Function Regularisation," and it consists precisely of introducing regularisation parameters that cause a divergent sum such as (5.307) to be replaced by $\sum_{n\ge 1} n^{-s}$. The regularisation scheme (whose rigour can be proved up to the "industry standards" of the subject) then consists of replacing the infinite result for $\sum_{n\ge 1} 1$ by the expression $\zeta(0)$, where $\zeta(s)$ is the analytically-continued function defined in (5.300).

The Riemann zeta function is very important also in number theory. This goes beyond the scope of this course, but a couple of remarks on the subject are may be of interest. First, we may make the following manipulation, valid for $\mathrm{Re}(s) > 1$:

$$\begin{aligned}
\zeta(s) &= \sum_{n\ge 1} n^{-s} = 1^{-s} + 2^{-s} + 3^{-s} + 4^{-s} + 5^{-s} + 6^{-s} + 7^{-s} + \cdots \\
&= 1^{-s} + 3^{-s} + 5^{-s} + \cdots + 2^{-s}\,(1^{-s} + 2^{-s} + 3^{-s} + \cdots) \\
&= 1^{-s} + 3^{-s} + 5^{-s} + \cdots + 2^{-s}\,\zeta(s)\,, \qquad (5.308)
\end{aligned}$$

whence

$$(1 - 2^{-s})\,\zeta(s) = 1^{-s} + 3^{-s} + 5^{-s} + \cdots\,. \qquad (5.309)$$

So all the terms where n is a multiple of 2 are now omitted in the sum. Now, repeat this excercise but pulling out a factor of 3^{-s}:

$$\begin{aligned}
(1 - 2^{-s})\,\zeta(s) &= 1^{-s} + 5^{-s} + 7^{-s} + 11^{-s} + \cdots + 3^{-s}\,(1^{-s} + 3^{-s} + 5^{-s} + 7^{-s} + \cdots)\,, \\
&= 1^{-s} + 5^{-s} + 7^{-s} + 11^{-s} + \cdots + 3^{-s}\,(1 - 2^{-s})\,\zeta(s)\,, \qquad (5.310)
\end{aligned}$$

whence

$$(1 - 2^{-s})\,(1 - 3^{-s})\,\zeta(s) = 1^{-s} + 5^{-s} + 7^{-s} + 11^{-s} + \cdots\,. \qquad (5.311)$$

We have now have a sum where all the terms where n is a multiple of 2 or 3 are omitted. Next, we do the same for factors of 5, then 7, then 11, and so on. If $2, 3, 5, 7, \ldots, p$ denote all the prime numbers up to p, we shall have

$$(1 - 2^{-s})\,(1 - 3^{-s}) \cdots (1 - p^{-s})\,\zeta(s) = 1 + {\sum}' n^{-s}\,, \qquad (5.312)$$

where $\sum'$ indicates that only those values of n that are prime to $2, 3, 5, 7, \ldots, p$ occur in the summation. It is now straightforward to show that if we send p to infinity, this summation goes to zero, since the "first" term in the sum is the lowest integer that is prime to all the primes, i.e. $n = \infty$. Since $\mathrm{Re}(s) > 1$, the "sum" is therefore zero. Hence we arrive at the result, known as *Euler's product* for the zeta function:

$$\frac{1}{\zeta(s)} = \prod_p \Big(1 - \frac{1}{p^s}\Big)\,, \qquad \mathrm{Re}(s) > 1\,, \qquad (5.313)$$

where the product is over all the prime numbers. This indicates that the Riemann zeta function can play an important rôle in the study of prime numbers.

We conclude this section with an application of the technique we discussed in section 5.8, for summing infinite series by contour integral methods. It is relevant to the discussion of the zeros of the Riemann zeta function. Recall that we showed previously that the zeta function could be represented by the integral (5.300), which we repeat here:

$$\zeta(s) = -\frac{\Gamma(1-s)}{2\pi\,\mathrm{i}} \int_C \frac{(-z)^{s-1}\,dz}{e^z - 1}\,, \tag{5.314}$$

where C is the Hankel contour. Now, imagine making a closed contour C', consisting of a large outer circle, centred on the origin, and with radius $(2N+1)\,\pi$, which joins onto the Hankel contour way out to the east in the complex plane. See Figure 9 below. As we observed previously, the integrand in (5.314) has poles at $z = 2\pi\,\mathrm{i}\,n$ for all the integers n. In fact, of course, it is very similar to the cosec and cot functions that we have been considering in our discussion in this section, since

$$\frac{1}{e^z - 1} = \frac{e^{-\frac{1}{2}z}}{e^{\frac{1}{2}z} - e^{-\frac{1}{2}z}} = \tfrac{1}{2} e^{-\frac{1}{2}z}\,\mathrm{cosech}\,(\tfrac{1}{2}z)\,. \tag{5.315}$$

The only difference is that because we now have the hyperbolic function cosech rather than the trigonometric function cosec, the poles lie along the imaginary axis rather than the real axis.

Since the Hankel contour itself was arranged so as to sneak around the origin without encompassing the poles at $z = \pm 2\pi\,\mathrm{i}, \pm 4\pi\,\mathrm{i}, \ldots$, it follows that the closed contour C' will precisely enclose the poles at $z = 2\pi\,\mathrm{i}\,n$, for all non-vanishing positive and negative integers n. For some given positive integer m, consider the pole at

$$z = 2\pi\,\mathrm{i}\,m = 2\pi\, e^{\frac{1}{2}\pi\,\mathrm{i}}\, m\,. \tag{5.316}$$

When we evaluate the residue $\mathcal{R}_m$ here, we therefore have

$$\mathcal{R}_m = (2\pi\, e^{-\frac{1}{2}\pi\,\mathrm{i}}\, m)^{s-1}\,, \tag{5.317}$$

since $(e^z - 1)^{-1}$ itself clearly has a simple pole with residue 1 there. (We have used the fact that (5.316) implies $-z = 2\pi\, m\, e^{-\frac{1}{2}\pi\,\mathrm{i}}$, since we have to be careful when dealing with the multiply-valued function $(-z)^{s-1}$.) There is also a pole at $z = -2\pi\, e^{\frac{1}{2}\pi\,\mathrm{i}}\, m$, which by similar reasoning will have the residue $\mathcal{R}_{-m}$ given by

$$\mathcal{R}_{-m} = (2\pi\, e^{\frac{1}{2}\pi\,\mathrm{i}}\, m)^{s-1}\,, \tag{5.318}$$

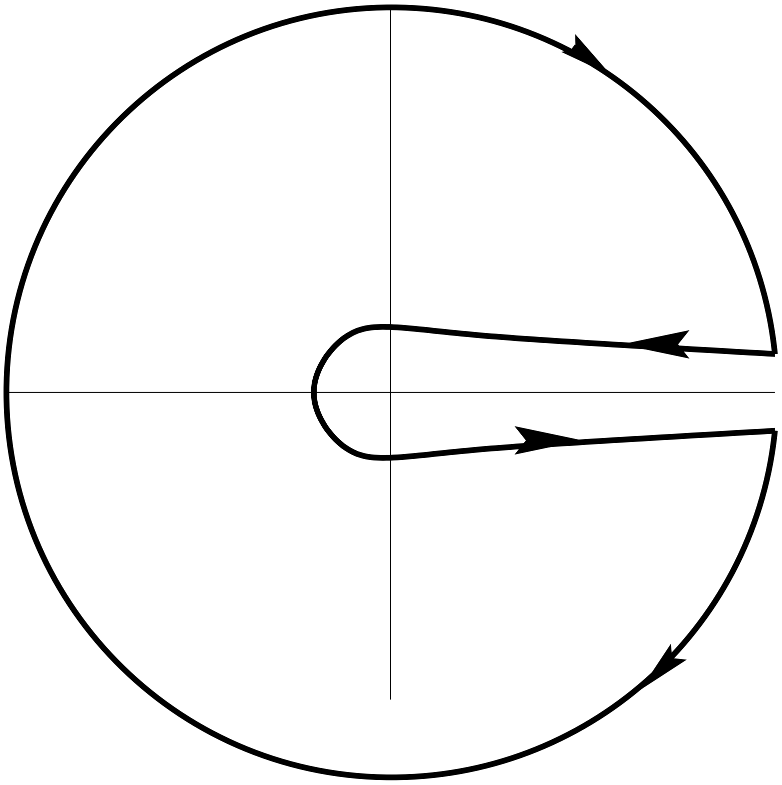

Figure 9: The contour C' composed of the Hankel contour plus a large circle

Putting the two together, we therefore get

$$\mathcal{R}_m + \mathcal{R}_{-m} = 2\,(2\pi\, m)^{s-1}\,\sin(\tfrac{1}{2}\pi\, s)\,. \tag{5.319}$$

By the theorem of residues, it follows that if we evaluate

$$\int_{C'} \frac{(-z)^{s-1}\,dz}{e^z - 1}\,, \tag{5.320}$$

where C' is the closed contour defined above, and then we send the radius $(2N+1)\pi$ of the outer circle to infinity, we shall get

$$\begin{aligned}\int_{C'} \frac{(-z)^{s-1}\,dz}{e^z - 1} &= -2\pi\,\mathrm{i}\sum_{m\ge 1}(\mathcal{R}_m + \mathcal{R}_{-m})\,,\\ &= -4\pi\,\mathrm{i}\sum_{m\ge 1}(2\pi\, m)^{s-1}\,\sin(\tfrac{1}{2}\pi\, s)\\ &= -2\,(2\pi)^s\,\mathrm{i}\,\sin(\tfrac{1}{2}\pi\, s)\sum_{m\ge 1} m^{s-1}\,,\\ &= -2\,(2\pi)^s\,\mathrm{i}\,\sin(\tfrac{1}{2}\pi\, s)\,\zeta(1-s)\,. \end{aligned} \tag{5.321}$$

It is clear from the final step that we should require $\mathrm{Re}(s) < 0$ here. (Note that the direction of the integration around large circle is *clockwise*, which is the direction of decreasing phase, so we pick up the extra -1 factor when using the theorem of residues.)

Now, if we consider the closed contour C' in detail, we find the following. It is comprised of the sum of the Hankel contour, plus the circle at large radius $R = (2N+1)\,\pi$, with N sent to infinity. On the large circle we shall have

$$|(-z)^{s-1}| = R^{s-1}\,, \tag{5.322}$$

which falls off faster than $1/R$ since we are requiring $\mathrm{Re}(s) < 0$. This is enough to outweigh the factor of R that comes from writing $z = R\,e^{\mathrm{i}\,\theta}$ on the large circle. Since the $(e^z - 1)^{-1}$ factor cannot introduce any divergence (the radii $R = (2N+1)\,\pi$ are cleverly designed to avoid passing through the poles of $(e^z-1)^{-1}$), it follows that the contribution from integrating around the large circle goes to zero as N is sent to infinity. Therefore when evaluating the contour integral on the left-hand side of (5.321), we are left only with the contribution from the Hankel contour C. But from (5.314), this means that we have

$$\int_{C'} \frac{(-z)^{s-1}\,dz}{e^z - 1} = \int_C \frac{(-z)^{s-1}\,dz}{e^z-1} = -\frac{2\pi\,\mathrm{i}}{\Gamma(1-s)}\,\zeta(s)\,. \tag{5.323}$$

Comparing with (5.321), we therefore conclude that if $\mathrm{Re}(s) < 0$,

$$\zeta(s) = 2\,(2\pi)^{s-1}\,\Gamma(1-s)\,\sin(\tfrac12\pi s)\,\zeta(1-s)\,. \tag{5.324}$$

This can be neatened up using the reflection formula (5.285) to write $\Gamma(1-s) = \pi/(\Gamma(s)\,\sin(\pi s))$, and then using the fact that $\sin(\pi s) = 2\sin(\frac12\pi s)\,\cos(\frac12\pi s)$. This gives us the final result

$$2^{s-1}\,\Gamma(s)\,\zeta(s)\,\cos(\tfrac12\pi s) = \pi^s\,\zeta(1-s)\,, \tag{5.325}$$

Both sides are analytic functions, except at isolated poles, and so even though we derived the result under the restriction $\mathrm{Re}(s) < 0$, it immediately follows by analytic continuation that it is valid in the whole complex plane. This beautiful formula was discovered by Riemann.

There is a very important, and still unproven conjecture, known as *Riemann's Hypothesis.* This concerns the location of the zeros of the zeta function. One can easily see from Euler's product (5.313), or from the original series definition (5.290), that $\zeta(s)$ has no zeros for $\mathrm{Re}(s) > 1$. One can also rather easily show, using Riemann's formula that we derived above, that when $\mathrm{Re}(s) < 0$ the only zeros lie at the negative even integers, $s = -2, -4, \ldots$. This leaves the strip $0 \le \mathrm{Re}(s) \le 1$ unaccounted for. Riemann's Hypothesis, whose proof would have far-reaching consequences in number theory, is that in this strip, all the zeros of $\zeta(s)$ lie on the line $\mathrm{Re}(s) = \frac12$.

Let us use Riemann's formula to prove the result stated above, namely that for $\mathrm{Re}(s) < 0$ the only zeros of $\zeta(s)$ lie at the negative even integers, $s = -2, -4 \ldots$. To do this, we need only observe that taking $\mathrm{Re}(s) > 1$ in (5.325), the functions making up the left-hand side are non-singular. Furthermore, in this region the left-hand side is non-zero except at the zeros of $\cos(\frac{1}{2}\pi\, s)$. (Since $\Gamma(s)$ and $\zeta(s)$ are both, from their definitions, clearly non-vanishing in this region.) In this region, the zeros of $\cos(\frac{1}{2}\pi\, s)$ occur at $s = 2n+1$, where n is an integer with $n \ge 1$. They are simple zeros. Thus in this region the right-hand side of (5.325) has simple zeros at $s = 2n + 1$. In other words, $\zeta(s)$ has simple zeros at $s = -2, -4, -6, \ldots$, and no other zeros when $\mathrm{Re}(s) < 0$.

Combined with the observation that the original series definition (5.290) makes clear that $\zeta(s)$ cannot vanish for $\mathrm{Re}(s) > 1$, we arrive at the conclusion that any possible additional zeros of $\zeta(s)$ must lie in the strip with $0 \le \mathrm{Re}(s) \le 1$. Riemann's formula does not help us in this strip, since it reflects it back onto itself. It is known that there are infinitely many zeros along the line $\mathrm{Re}(s) = \frac{1}{2}$. As we mentioned before, the still-unproven *Riemann Hypothesis* asserts that there are no zeros in this strip except along $\mathrm{Re}(s) = \frac{1}{2}$.

5.12 Asymptotic Expansions

Until now, whenever we have made use of a series expansion for a function it has been taken as axiomatic that the series should be *convergent* in order to be usable, since a diverging series obviously, by definition, is giving an infinite or ill-defined result. Surprisingly, perhaps, there are circumstances where a diverging series is nevertheless useful. The basic idea is that even if the series has a divergent sum, it might be that by stopping the summation at some appropriate point, the partial summation can give a reasonable approximation to the required function. An series of this sort is known as an *Asymptotic Expanson.*

First, let us look at an illustrative example. Consider the function $f(x)$ defined by

$$f(x) = e^x \int_x^\infty t^{-1}\, e^{-t}\, dt\,. \tag{5.326}$$

Integrating by parts we get

$$\begin{aligned} f(x) &= e^x \Big[-t^{-1}\, e^{-t}\Big]_x^\infty - e^x \int_x^\infty t^{-2}\, e^{-t}\, dt\,,\\ &= \frac{1}{x} - e^x \int_x^\infty t^{-2}\, e^{-t}\, dt\,. \end{aligned} \tag{5.327}$$

Integrating by parts n times gives

$$f(x) = \frac{1}{x} - \frac{1}{x^2} + \frac{2!}{x^3} - \frac{3!}{x^4} + \cdots + \frac{(-1)^{n+1}\,(n-1)!}{x^n} + (-1)^n\, n!\, e^x \int_x^\infty t^{-n-1}\, e^{-t}\, dt\,. \tag{5.328}$$

This seems to be giving us a nice series expansion for $f(x)$. The only trouble is that is is divergent.

If we define

$$u_{n-1} \equiv \frac{(-1)^n\,(n-1)!}{x^n}\,, \tag{5.329}$$

then we would have

$$f(x) = \sum_{n=0}^{\infty} u_n \tag{5.330}$$

if the series expansion made sense. If we apply the ratio test for convergence, we find

$$\Big|\frac{u_m}{u_{m-1}}\Big| = \frac{m}{x}\,, \tag{5.331}$$

which goes to infinity as m goes to infinity, at fixed x. Thus the radius of convergence is zero.

Rather than abandoning the attempt, consider the partial sum

$$S_n(x) \equiv \sum_{m=0}^{n} u_m = \frac{1}{x} - \frac{1}{x^2} + \frac{2!}{x^3} - \cdots + \frac{(-1)^n\,n!}{x^{n+1}}\,. \tag{5.332}$$

Now let us compare $S_n(x)$ with $f(x)$. From (5.328), we have

$$f(x) - S_n(x) = (-1)^{n+1}\,(n+1)!\,e^x \int_x^\infty t^{-n-2}\,e^{-t}\,dt = (-1)^{n+1}\,(n+1)! \int_x^\infty t^{-n-2}\,e^{x-t}\,dt\,. \tag{5.333}$$

Using the fact that $e^{x-t} \le 1$ for $x \le t \le \infty$, we therefore have

$$|f(x) - S_n(x)| < (n+1)! \int_x^\infty t^{-n-2}\,dt = \frac{n!}{x^{n+1}}\,. \tag{5.334}$$

We see that if we take x to be sufficiently large, whilst holding n fixed, then (5.334) becomes very small. This means that the partial sum $S_n(x)$ will be a good approximation to $f(x)$ if we take x sufficiently large. Furthermore, the larger we choose x to be, the larger we can take n to be. So by taking n to be large (implying that x will need to be very large), we see that we can make $|f(x) - S_n(x)|$ to be very small indeed. The function $f(x)$ can be calculated to high accuracy for large x by taking the sum of a suitable number of terms in the series $\sum_m u_m$. This is known as an asymptotic expansion of $f(x)$. It is usually denoted by the symbol $\sim$ rather than an equals sign, namely

$$f(x) \sim \sum_{m=1}^{\infty} \frac{(-1)^m\,(m-1)!}{x^m}\,. \tag{5.335}$$

A precise definition of an asymptotic expansion is the following. A divergent series

$$a_0 + \frac{a_1}{z} + \frac{a_2}{z^2} + \cdots + \frac{a_n}{z^n} + \cdots \tag{5.336}$$

in which the sum of the first $(n+1)$ terms is $S_n(z)$ is said to be an asymptotic expansion of a function $f(z)$ (for some specified range of values for $\arg(z)$) if the quantity $R_n(z) \equiv z^n\,(f(z) - S_n(z))$ satisfies

$$\lim_{|z| \longrightarrow \infty} R_n(z) = 0 \qquad (n \text{ fixed})\,, \tag{5.337}$$

even though

$$\lim_{n \longrightarrow \infty} |R_n(z)| = \infty \qquad (z \text{ fixed})\,, \tag{5.338}$$

This last equation is the statement that the series is divergent, whilst (5.337) is the statement that the series is usable in the asymptotic sense. In other words, we can ensure that

$$|z^n\,(f(z) - S_n(z))| < \epsilon \tag{5.339}$$

for any arbitrarily small ϵ, by taking $|z|$ to be sufficiently large.

It is easy to see that our original example (5.335) satisfies the condition (5.337), since from (5.334) we have

$$|x^n\,(f(x) - S_n(x))| < \frac{n!}{x} \longrightarrow 0 \qquad \text{as} \qquad x \longrightarrow \infty\,. \tag{5.340}$$

Notice that unlike ordinary convergent series expansions, an asymptotic expansion is not unique; it is possible for two *different* functions to have an identical asymptotic expansion. An equivalent statement is that there exist functions whose asymptotic expansion is simply 0. An example of such a function is

$$f(x) = e^{-x}\,, \tag{5.341}$$

when x is positive. It is clear that this function itself satisfies the condition (5.337), for any n:

$$x^n\,e^{-x} \longrightarrow 0 \qquad \text{as} \qquad x \longrightarrow \infty\,, \tag{5.342}$$

and so the appropriate asymptotic expansion for e^{-x} is simply

$$e^{-x} \sim 0\,. \tag{5.343}$$

Of course, having established that there exist functions whose asymptotic expansion is 0, it is an immediate consequence that adding such a function to any function $f(x)$ gives another with the same asymptotic expansion as $f(x)$.

It is important to know the rules about what is allowable, and what is not allowable, when performing manipulations with asymptotic expansions. Firstly, if two asymptotic expansions that are valid in an overlapping range of values of $\arg(z)$ are multiplied together, then the result is an asymptotic expansion for the product of the two functions they represented. Thus if

$$f(z) \sim \sum_{n=0}^{\infty} a_n\, z^{-n} \qquad \text{and} \qquad g(z) \sim \sum_{n=0}^{\infty} b_n\, z^{-n}\,, \tag{5.344}$$

then

$$f(z)\, g(z) \sim \sum_{n=0}^{\infty} c_n\, z^{-n}\,, \tag{5.345}$$

where

$$c_n = \sum_{p=0}^{n} a_p\, b_{n-p}\,. \tag{5.346}$$

In other words, one just multiplies the expansions in the ordinary way, and, *qua* asymptotic expansions, the results behave as one would hope. One proves this by directly verifying that the condition (5.337) is satisfied by (5.345).

Another allowed manipulation is the integration of an asymptotic expansion. For example, if we have an asymptotic expansion

$$f(x) \sim \sum_{n=2}^{\infty} a_n\, x^{-n}\,, \tag{5.347}$$

then integrating this term by term gives an asymptotic expansion for the integral of $f(x)$:

$$\begin{aligned} \int_x^{\infty} f(y)\, dy \quad &\sim \quad \sum_{n=0}^{\infty} a_n \int_x^{\infty} y^{-n}\, dy \\ &\sim \quad \sum_{n=2}^{\infty} \frac{1}{n-1}\, a_n\, x^{-n+1}\,. \end{aligned} \tag{5.348}$$

(We considered an example where $a_0 = a_1 = 0$, for the sake of minor simplification of the discussion.) Again, the proof of this statement is a simple matter of verifying that the condition (5.337) for an asymptotic expansion is satisfied.

The situation for differentiation of an asymptotic expansion is a little more complicated. It is not in general permissable to differentiate an asymptotic expansion for $f(x)$, unless it is already known by some other means that $f'(x)$ itself has an asymptotic expansion. An example that illustrates this is $f(x) = e^{-x}\, \sin(e^x)$. This function is similar to e^{-x}, in that its asymptotic expansion for positive x is simply 0:

$$f(x) = e^{-x}\, \sin(e^x) \sim 0\,. \tag{5.349}$$

(It is easy to see that $x^n\, e^{-x}\, \sin(e^x)$ goes to zero as x goes to $+\infty$, for any n. This is because the e^{-x} goes to zero faster than any power of x as x goes to infnity, while $|\sin(e^x)| \le 1$.)

However, the derivative of $f(x)$ is

$$f'(x) = -e^{-x} \sin(e^x) + \cos(e^x)\,, \tag{5.350}$$

and the second term does not admit an asymptotic expansion.

Notice that in our discussion of asymptotic expansions, the phase of z, i.e. $\arg(z)$, plays an important rôle. A function $f(z)$ may have a totally different asymptotic expansion for some range of $\arg(z)$ as compared with some other range. For example, we saw that the function e^{-x} has the asymptotic expansion $e^{-x} \sim 0$ when x is real and positive. On the other hand, if x is real and negative, it is easily verified that it does not admit any asymptotic expansion at all. In less extreme examples, one can encounter functions that have "interesting" but different asymptotic expansions for different ranges of $\arg(z)$.

A common situation where asymptotic expansions arise occurs in a particular kind of approximation scheme for evaluating certain classes of contour integral, known as the "Method of Steepest Descent." It is to this subject that we now turn.

5.13 Method of Steepest Descent

This approximation scheme is applicable to a certain rather special class of contour integral, of the following form:

$$J(s) = \int_C g(z)\, e^{s\, f(z)}\, dz\,. \tag{5.351}$$

The idea is that one wants to get an approximate asymptotic form for $J(s)$, valid for large values of s. For now, we shall have in mind that s is real. The method assumes that the function $f(z)$ is such that its real part goes to $-\infty$ at both ends of the contour C. It is furthermore assumed that the prefactor function $g(z)$ is a slowly-varying one, so that the behaviour of the integrand is dominated by the exponential factor. In particular, the integrand will be assumed to vanish (for positive real s), at both endpoints.

If the parameter s is large and positive, the integrand will become large when the real part of $f(z)$ is large and positive, and on the other hand the integrand will become relatively small when the real part of $f(z)$ is small or negative. If we are seeking to approximate $J(s)$ by an asymptotic expansion, then we are interested in the situation when s becomes arbitrarily large and positive. It is clear then that the asymptotic behaviour of $J(s)$ will be dominated from the contribution (or contributions) to the integral from the region or (regions) where the real part of $f(z)$ reaches a maximum value.

Within reason, we are allowed to deform the integration path C as we wish, without affecting the final result for $J(s)$. Specifically, provided the deformation does not cause the path to cross over a pole or other singularity of the integrand, then we can distort the path in any desired way. As we have observed above, the most important contributions to $J(s)$ will come from the place or places along the path where the real part of the function $f(z)$ has a maximum. Let us assume for now, to simplify the discussion, that there is just one such maximum, at $z = z_0$. Thus at this point we shall have $\partial u/\partial x = 0 = \partial u/\partial y$, and hence

$$f'(z_0) = 0 \,. \tag{5.352}$$

If we consider integrating along the segment of the contour in the vicinity of the maximum at $z = z_0$, it is clear that life would be made a lot simpler if it were the case that the imaginary part of $f(z)$ were constant there. To see this, write $f(z) = u(x,y) + \mathrm{i}\, v(x,y)$. If the imaginary part $v(x,y)$ were varying along the path near $z = z_0$, then when s is very large it is clear that there will be a factor

$$e^{\mathrm{i}\, s\, v} \tag{5.353}$$

in the integrand that is making the phase spin round and round like a propeller blade. Evaluating the integral along this dominant segment of the whole path C would then be very tricky.

To avoid this difficulty, we can exploit our freedom to deform the integration path, so that we angle it around in the neighbourhood of $z = z_0$ such that $v(x,y)$ is nearly constant there. So we want our path near $z = z_0$ to be such that both of the following conditions hold:

$$f'(z_0) = 0 \,, \qquad \mathrm{Im}(f(z)) = \mathrm{Im}(f(z_0)) \,. \tag{5.354}$$

Now early on in our discussion of analytic functions, we saw that the real and imaginary parts satisfy the following equations:

$$\nabla^2 u = 0 = \nabla^2 v \,, \qquad \nabla u \cdot \nabla v = 0 \,. \tag{5.355}$$

The first of these two conditions tells us that u and v cannot have maxima or minima. Thus, to take u for example, it tells us that

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \,. \tag{5.356}$$

So if the second derivative with respect to x is positive at some point, then the second derivative with respect to y must be negative there. So the stationary point $z = z_0$ that we defined by our requirement $f'(z_0) = 0$ must actually be a *saddle point*. When we speak of $z = z_0$ corresponding to the maximum of $u(x,y)$ on our path, we should therefore have in mind the image of a hiker slogging up to a mountain pass, or saddle, and heading on down the other side. As he reaches the top of the saddle, he actually sees the ground rising both to his left and to his right, but he, having attained the saddle, heads on downwards into the valley on the other side.

Now consider the second equation in (5.355). This says that the lines of u=constant are orthogonal to the lines of v =constant. Therefore, if you try to imagine the topography in the vicinity of the saddle, this means that the way to keep v =constant as you walk up and over the saddle is to make sure that you choose your path such that u falls off as rapidly as possible, on either side of the saddle peak. Thus, viewing your path from the top of the saddle, it should descend as rapidly as possible into the valley on either side. In other words, the contour should follow the path of *Steepest Descent*.

We shall therefore now assume that we have adjusted the contour so that either side of the point z_0, it follows the steepest possible path of decreasing $u(x, y)$. Near $z = z_0$, we necessarily have that

$$f(z) = f(z_0) + \tfrac{1}{2}(z - z_0)^2 \, f''(z_0) + \cdots \,, \tag{5.357}$$

since we defined z_0 by $f'(z_0) = 0$. Since the contour has the property that v =constant, it follows that $\frac{1}{2}(z - z_0)^2 \, f''(z_0)$ must be real. Furthermore, it must be negative along the contour, since by construction the contour is such that u decreases in each direction as one moves away from $z = z_0$. Then, assuming $f''(z_0) \neq 0$, we have

$$f(z) - f(z_0) \approx \tfrac{1}{2}(z - z_0)^2 \, f''(z_0) = -\frac{1}{2s} \, t^2 \,, \tag{5.358}$$

where this equation is defining the new (real) variable t.

As we have already observed, since we are assuming that s is large and positive, the integral will be dominated by the contribution from the region near to $z = z_0$. We are assuming also that $g(z)$ is slowly varying, so to a good approximation we may take it outside the integration, setting its argument equal to z_0, and hence we shall have the approximate result that

$$J(s) \approx g(z_0) \, e^{s \, f(z_0)} \int_{-\infty}^{\infty} e^{-\frac{1}{2} t^2} \, \frac{dz}{dt} \, dt \,. \tag{5.359}$$

Note that we have taken the range of the integration to run from $-\infty$ to ∞. Again, this is an approximation that is well justified when s is large and positive. This can be seen by looking at (5.358): When s is very large, t can become very large before the magnitude of $f(z) - f(z_0)$ becomes appreciable. In other words, by the time the approximation of expanding $(f(z) - f(z_0)$ as in (5.358) has broken down the value of t is so large that $e^{-\frac{1}{2} t^2}$

is negligable, and so the error introduced by allowing t to run all the way out to $\pm\infty$ is very small.

To complete the evaluation of the integral, we just need to work out dz/dt. Near to $z = z_0$, we may write

$$z - z_0 = q\, e^{\mathrm{i}\,\alpha}\,, \tag{5.360}$$

where q is real and the phase α is constant. In fact α specifies the angle in the complex plane along which the direction of steepest descent lies. Thus from (5.358) we have

$$t^2 = -s\, f''(z_0)\, q^2\, e^{2\mathrm{i}\,\alpha}\,, \tag{5.361}$$

and therefore

$$t = q\, |s\, f''(z_0)|^{\frac{1}{2}}\,. \tag{5.362}$$

This means that we can write

$$\frac{dz}{dt} = e^{\mathrm{i}\,\alpha}\, \frac{dq}{dt} = e^{\mathrm{i}\,\alpha}\, |s\, f''(z_0)|^{-\frac{1}{2}}\,, \tag{5.363}$$

implying from (5.359) that

$$J(s) \sim \frac{g(z_0)\, e^{s\, f(z_0)}\, e^{\mathrm{i}\,\alpha}}{|s\, f''(z_0)|^{\frac{1}{2}}} \int_{-\infty}^{\infty} e^{-\frac{1}{2}t^2}\, dt\,. \tag{5.364}$$

The remaining integral here is just a Gaussian, giving a factor $\sqrt{2\pi}$, and so we arrive at the final result

$$J(s) \sim \frac{\sqrt{2\pi}\, g(z_0)\, e^{s\, f(z_0)}\, e^{\mathrm{i}\,\alpha}}{|s\, f''(z_0)|^{\frac{1}{2}}}\,. \tag{5.365}$$

Note that we have written this using the symbol $\sim$, denoting an asymptotic expansion. This is indeed appropriate; it is an approximation that gets better and better as s gets larger and larger.

An it is instructive to look at an example at this point. Let us consider the Gamma function $\Gamma(s+1)$, which can be expressed in terms of the integral representation (5.267):

$$\Gamma(s+1) = \int_0^\infty x^s\, e^{-x}\, dx\,. \tag{5.366}$$

(We consider $\Gamma(s+1)$ here purely for later convenience; blame Euler, as usual, for the shift by 1!) First, we make the substitution $x = s\, z$, so that in terms of the new integration variable z we shall have

$$\Gamma(s+1) = s^{s+1} \int_0^\infty z^s\, e^{-s\, z}\, dz = s^{s+1} \int_0^\infty e^{s\,(\log z - z)}\, dz\,. \tag{5.367}$$

Writing it in this way, we see that it indeed has the general form off (5.351), with $g(z) = 1$ and

$$f(z) = \log z - z\,. \tag{5.368}$$

The contour here is along the real axis, so z is in fact just a real variable here. It is clear that $f(z)$ does indeed go to $-\infty$ at both endpoints of the integration, namely at $z = 0$ and $z = \infty$.

To apply the method of steepest descent to this example, we first locate the stationary point of $f(z)$, by solving $f'(z) = 1/z - 1 = 0$, giving $z_0 = 1$. We also need to calculate $f''(z) = -1/z^2$ at $z = z_0 = 1$, giving $f''(1) = -1$. There is no need to perform any deformation of the original contour in this example, since the imaginary part of $f(z)$ is zero in the whole region (for real z) around $z = z_0 = 1$. Furthermore, the phase α vanishes. Substituting into (5.365), we therefore obtain the result

$$\Gamma(s+1) \sim \sqrt{2\pi}\, s^{s+\frac{1}{2}}\, e^{-s}\,. \tag{5.369}$$

Recalling that $\Gamma(s+1)$ is otherwise known as $s!$, we can recognise (5.369) as *Stirling's Approximation* to the factorial function.

How good an approximation is (5.369)? Well, we expect that it should get better and better as s gets larger and larger. A tabulation of the actual values and the results from Stirling's approximation, for a variety of values of s is instructive. This is given below in Table 1. We see that Stirling's approximation to the Gamma function rapidly becomes quite a good one, even for quite modest values of s.

We have seen that the methods of steepest descents has given a useful approximation to the Gamma function, and in a similar way it can be used in many other examples too. One might worry that, as presented above, it seems to be a method that produces a specific approximate expression, without any indication of how to get a better one by pushing things to higher orders. In fact, the approximations we made in the derivation above are nothing but the leading-order terms in a series expansion that can be developed and pushed, in principle, to arbitrary order. Not surprisingly, the series expansion that one obtains by this method is an asymptotic expansion, and not a convergent series.

To see how we develop the full series, let us go back to the Taylor expansion (5.357) for $f(z)$, which we approximated by just retaining the leading-order term, as in (5.358). All that we need do in order to get the full asymptotic series for $J(s)$ is to work with the exact expression, rather than the approximation in (5.358). Thus we define t not by (5.358), but instead by

$$f(z) - f(z_0) = -\frac{1}{2s}\, t^2\,. \tag{5.370}$$

We use this expession in order to substitute for dz/dt in (5.359). Of course this is generally easier to say than to do, since one effectively has to invert the expression (5.370) in order to obtain z as a function of t. Usually, one has to do this at the level of a power-series expansion.

One can easily write (5.370) as a power series, giving t as an expansion in powers of z. There is in fact a systematic way to invert such a series, so that one obtains instead z as a power series in t. It can be derived most elegantly using the calculus of residues. We shall not interrupt the flow of this discussion to describe this here. Instead. let us take our previous discussion of the Stirling approximation for the Gamma function, and push it to a couple more orders by doing a somewhat brute-force inversion of the relevant power series.

Recall that for the Gamma function we had $f(z) = \log z - z$, and hence the stationary point $f'(z_0) = 0$ determines that $z_0 = 1$. Thus from (5.370) we have

$$(z-1) - \log[1 + (z-1)] = \frac{1}{2s} t^2\,. \tag{5.371}$$

The left-hand side here can be expanded in a power series in $w \equiv (z-1)$, around the point $w = 0$, giving

$$\tfrac{1}{2} w^2 - \tfrac{1}{3} w^3 + \tfrac{1}{4} w^4 - \tfrac{1}{5} w^5 + \cdots = \frac{1}{2s}\, t^2\,. \tag{5.372}$$

We must now recast this as an expression for w as a power series in t. Thus we seek to write it as

$$w = \sum_{n\ge 0} a_n\, t^n\,. \tag{5.373}$$

We can determine the coefficients a_n simply by inserting (5.373) into (5.371), expanding in powers of t, and solving order by order for the a_n such that it equal $t^2/(2s)$, as demanded by (5.372). The result for the first few orders is

$$z - 1 = w = \frac{t}{s^{\frac{1}{2}}} + \frac{t^2}{3s} + \frac{t^3}{36 s^{\frac{3}{2}}} - \frac{t^4}{270 s^2} + \frac{t^5}{4320 s^{\frac{5}{2}}} + \cdots\,. \tag{5.374}$$

Thus we have

$$\frac{dz}{dt} = \frac{1}{s^{\frac{1}{2}}} + \frac{2t}{3s} + \frac{t^2}{12 s^{\frac{3}{2}}} - \frac{2t^3}{135 s^2} + \frac{t^4}{864 s^{\frac{5}{2}}} + \cdots\,. \tag{5.375}$$

Substituting this into (5.359), it is clear by symmetry that only the terms in (5.375) that involve *even* powers of t will give non-zero contributions in the integral. The non-vanishing ones can be evaluated by means of simple integrations by parts, to reduce them to the standard Gaussian inetgral. Thus we see from (5.367) that we obtain

$$\Gamma(s+1) \sim \sqrt{2\pi}\, s^{s+\frac{1}{2}}\, e^{-s} \Big(1 + \frac{1}{12s} + \frac{1}{288s^2} + \cdots\Big)\,. \tag{5.376}$$

This series, which could in principle be developed to any arbitrary desired order, is the asymptotic expansion for the Gamma function.

Finally, it is interesting to see how a numerical comparison with the true function looks now.

s	$s!$	Stirling	Higher-order
0.01	0.994325851191	0.236999259660	10.44113405058
0.1	0.951350769867	0.569718714898	1.242303308874
1	1	0.922137008896	1.002183624251
10	$3.628800000000\ 10^{6}$	$3.598695618741\ 10^{6}$	$3.628809703606\ 10^{6}$
100	$9.3326215443944\ 10^{157}$	$9.324847625269\ 10^{157}$	$9.3326215694180\ 10^{157}$
1000	$4.023872600771\ 10^{2567}$	$4.023537292037\ 10^{2567}$	$4.023872600782\ 10^{2567}$

Table 1: Comparison of $s!$, Stirling's formula (5.369), and the higher-order expansion (5.376)

Looking at the various entries in this Table, we see that for large s the asymptotic expansion up to the order given in (5.376) is doing very well indeed. The Table also serves to illustrate the fact that at small values of s, the inclusion of higher terms in the asymptotic expansion in fact makes things worse, not better. This is exactly what we expected; for any given value of the argument there is an optimum place at which to cut off the series, and including terms beyond that will give a worse approximation. For very small s, where the asymptotic series is in any case expected to be a disaster, we indeed see that we can make it even worse by adding more terms.

6 Non-linear Differential Equations

Most of our discussion of differential equations in this course has been concerned with *linear* second-order ordinary differential equations, of the form

$$y''(x) + p(x)\, y'(x) + q(x)\, y(x) = 0\,. \tag{6.1}$$

It is not uncommon to encounter ordinary differential equations that are non-linear in the dependent variable y. In such cases, one may be lucky and discover that the equation can be solved analytically, possibly after spotting some clever changes of dependent or independent variable. More often than not, however, the equation may prove not to be susceptible to exact solution by analytic methods. If this is the case then one has to find some other way of studying the solutions. One approach is to use numerical methods, which usually means "putting it on the computer." This is very straightfoward these days, and many computer languages come equipped with packages for solving differential equations numerically. For example, the algebraic computing language *Mathematica* offers also functions that will solve essentially any given differential equation, or set of differential equations, numerically. Of course if the problem is of any complexity or subtlety, it probably pays to have a deeper understanding of exactly how the numerical routines work. This is a major and important subject, which lies outside the scope of this course.

Another approach that can prove to be very useful is to make use of graphical methods for studying the behaviour of the solutions to the differential equation. Such techniques can be very helpful for a variety of reasons. Firstly, they are rather simple and intuitive, allowing one to see the structure of the solutions without the need for detailed computation; the behaviour can often be established just with a few scribblings on the back of an envelope. Secondly, the graphical techniques can be very helpful for revealing the way in which the solutions depend upon the choice of initial conditions or boundary conditions.

To begin our discussion, let us consider first the rather simple case of first-order non-linear differential equations.

6.1 Method of Isoclinals

Let us consider the first-order differential equation

$$\frac{dy}{dx} = f(x,y)\,. \tag{6.2}$$

Solveing the differential equation means finding the *integral curves* in the (x, y) plane, namely the functions $y(x)$ that satisfy (6.2). For many choices of the function $f(x, y)$, it is impossible to obtain an analytic solution to the equation.

To analyse the solutions graphically, we begin by considering the algebraic equation

$$f(x,y) = \lambda\,, \tag{6.3}$$

where λ is an arbitrary constant. For each choice of λ, this equation defines a curve in the (x, y) plane.

Clearly, it must be that wherever a solution $y = y(x)$ to (6.2) crosses the curve (6.3), the gradient of the integral curve is simply given by λ, since we shall have

$$\frac{dy}{dx} = \lambda \tag{6.4}$$

at that point. Since each point on a given curve implies that the integral curve intersecting it has the same gradient λ, the curve $f(x, y) = \lambda$ is called an *isocline*, or an *isoclinal curve*.

If we plot the isoclinal curves $f(x, y) = \lambda$ for a range of values of λ, and draw little line segments on each curve, with gradient equal to λ, then if we simply "join the segments" with lines that intersect the $f(x, y) = \lambda$ curves with gradient λ, then the resulting lines will be the integral curves for (6.2). In other words, these lines will precisely describe the solutions to the differential equation. The various different lines correspond to the possible choices of initial condition, associated with the arbitrary constant of integration for (6.2).

Let us begin with a simple example, where we can actually solve the differential equation explicitly, so that we shall be able to see exactly what is going on. Consider the case where $f(x, y) = x + y$, for which we can easily solve (6.2), to give

$$y = c\, e^x - 1 - x\,, \tag{6.5}$$

where c is an arbitrary constant. We shall keep this at the back of our minds, but proceed for now with the graphical approach and then make a comparison with the actual solutions afterwards. The isoclinal curves are $x + y = \lambda$, or in other words,

$$y = -x + \lambda\,. \tag{6.6}$$

These are straight lines, themselves all having slope -1, with the constant λ parameterising the point of intersection of the isocline with the y axis. A few of them are plotted in Figure 10 below; for those with the benefit of colour they are in blue, but in any case they are recognisable as the straight lines running between the north-west and the south-east. Imagine little line segments intersecting with each isoclinal, with slopes equal to the λ value specifying the isoclinal. This λ value is equal to the intercept of the isoclinal with the y axis. Thus the isoclinal passing though $(0, 0)$ would be decorated with little line segments of slope 0; the isoclinal passing through $(0, 1)$ would be decorated with little line segments of slope 1, and so on.

Also depicted in Figure 10 are some of the integral curves, i.e. the actual solutions of the differential equation $y' = x + y$. Secretly, we know they are given by (6.5) (and ideed, that is how Figure 10 was actually constructed!), but we are pretending that we have to draw the integral curves by the method described above. Thus the strategy is to draw lines that intersect the isoclinals with slopes equal to the slopes of the little line-segment decorations described above. Looking at Figure 10, we see that indeed the integral curves all have this property. For example, it can be seen that wherever an integral curve intersects the isoclinal that passes through $(0,0)$, it has slope 0. And wherever an integral curve intersects the isoclinal passing through $(0,1)$, it has slope 1, and so on. (Observe that all the integral curves indeed intersect the $(0,1)$ isoclinal perpendicularly, as they shhould since they have slope $+1$ there, while the isoclinal itself has slope -1.)

A convenient way to characterise the integral curves in this example is by the value of y_0 where they intersect the y axis. Looking at our "secret" formula (6.5), this is related to the integration constant c by $y_0 = c - 1$. Of course we know from the general analysis that if we also draw in the isoclinal passing through $(0, y_0)$, it will be decorated by little line segments of slope y_0. So the integral curve that passes through $(0, y_0)$ has slope y_0 at that point. The complete integral curve can then be built up by "joining the dots," so that it intersects the isoclinals at the correct angles. Of course in practice one may need to draw quite a lot of isoclinals, especially in regions of the (x, y) plane where "interesting" things may be happening.

Note that in this toy example, on the left-hand side of the diagram all of the integral curves become asymptotic to the isoclinal passing through $(0,-1)$, as x tends to $-\infty$. This is because this isoclinal is decorated by little line segments of slope -1, i.e. parallel to the isoclinal itself. Thus it acts as a sort of "attractor" line, with all the integral curves homing in towards it as x gets more and more negative. Of course we can see this explicitly if we sneak another look at our "secret solution" (6.5); all the solutions at large negative x approach $y = -x - 1$, regardless of the value of c.

For a second example, consider the equation

$$\frac{dy}{dx} = x^2 + y^2 \,. \tag{6.7}$$

The isoclines are given by the equation $x^2 + y^2 = \lambda$, which defines circles of radius $\sqrt{\lambda}$ centred on the origin in the (x, y) plane. Each circle should be decorated with little line segments whose gradient is λ, so the larger the circle, the steeper the gradient. The circle of zero radius corresponds to gradient zero.

The isoclinal lines and the integral curves for this example are depicted in Figure 11 below.

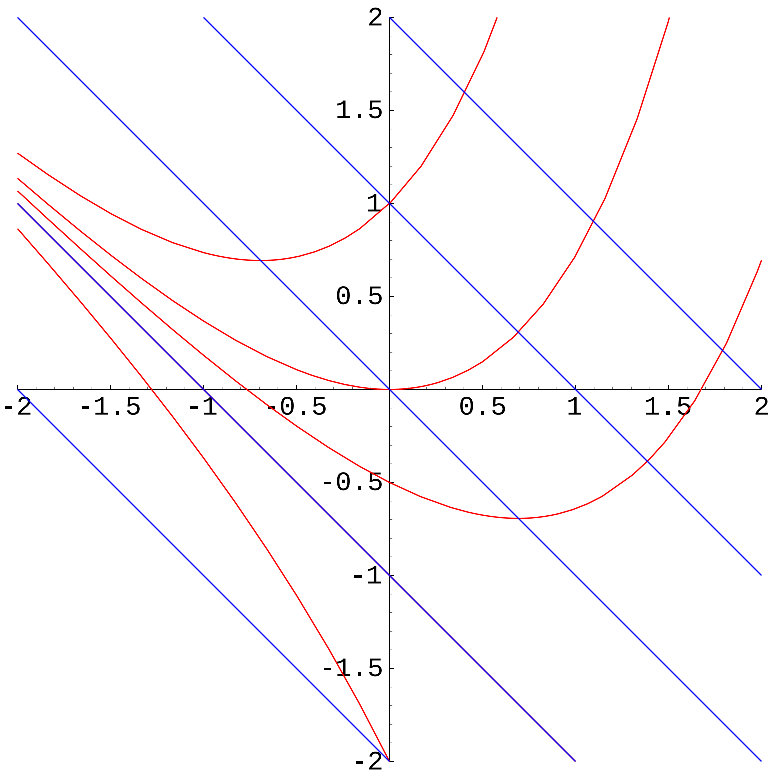

Figure 10: The isoclinal curves $y = -x + \lambda$ (displayed in blue), and the integral curves (displayed in red) for the differential equation $y' = x + y$.

Observe again that all the integral curves passing through a given isoclinal (the circles) do so with the same slope. And indeed, one can see that the as the circles get smaller, so the slope gets smaller.

The equation (6.7) in this example can in fact be solved explicitly, although it takes a form that is perhaps not immediately illuminating:

$$y = \frac{x\,(c J_{\frac{3}{4}}(\frac{1}{2}x^2) - J_{-\frac{3}{4}}(\frac{1}{2}x^2))}{c J_{-\frac{1}{4}}(\frac{1}{2}x^2) + J_{\frac{1}{4}}(\frac{1}{2}x^2)}\,, \tag{6.8}$$

where c is an arbitrary constant and $J_\nu(x)$ denotes the Bessel function of the first kind, which solves Bessel's equation $x^2\,J_\nu'' + x\,J_\nu' + (x^2 - \nu^2)\,J_\nu = 0$. It is quite useful, therefore, even in a case like this where there exists an explicit but complicated exact result, to be able to study the behaviour graphically. It is perhaps helpful to observe, since we do still have the luxury of having an analytic expression for the solution here, that the first couple of terms in its Taylor expansion around $x = 0$ are given by

$$y = \frac{-2\Gamma(\frac{3}{4})}{c\,\Gamma(\frac{1}{4})} + \frac{4\Gamma(\frac{3}{4})^2\,x}{c^2\,\Gamma(\frac{1}{4})^2} + \cdots\,. \tag{6.9}$$

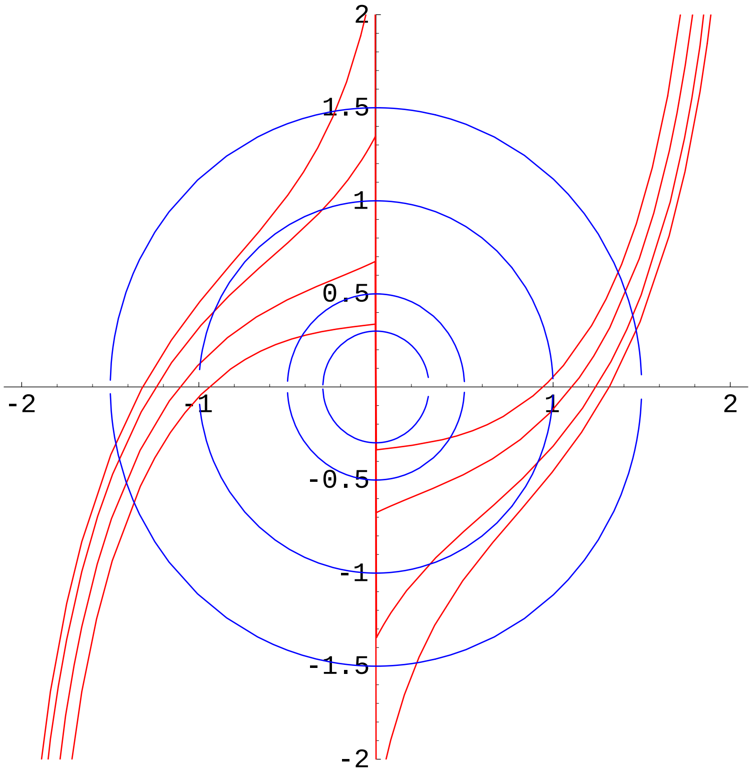

Figure 11: The isoclinal curves $y^2 = \lambda - x^2$ (displayed in blue), and the integral curves (displayed in red) for the differential equation $y' = x^2 + y^2$.

(This expansion is valid for x approaching zero from above. For negative x, the overall sign should be reversed. This follows from the fact, manifest in (6.8), that the solution is an odd function of x.)

6.2 Phase-plane Diagrams

The method of isoclinals described above applies specifically to first-order differential equations. We can make use of this technique in order to study graphically the solutions of a rather wide class of second-order ordinary differential equation. Specifically, if t is the independent variable and x the dependent variable, we can study any differential equation where all the terms are functions of x, $\dot{x}$ and $\ddot{x}$ only; in other words the independent variable t does not appear explicitly anywhere. Such differential equations are sometimes called *autonomous*. An example would be the *van de Pol equation*,

$$\ddot{x} - \epsilon\,(1 - x^2)\,\dot{x} + x = 0\,. \tag{6.10}$$

Any aoutonomous second-order ODE can be reduced to a first-order ODE. The trick is to define the quantity

$$y = \dot{x}\,, \tag{6.11}$$

from which it follows that

$$\ddot{x} = \frac{dy}{dt} = \frac{dx}{dt}\,\frac{dy}{dx} = y\,\frac{dy}{dx}\,. \tag{6.12}$$

Thus, in the example (6.10) above, the differential equation can be rewritten as

$$y\,\frac{dy}{dx} - \epsilon\,(1-x^2)\,y + x = 0\,. \tag{6.13}$$

Any autonomous second-order ordinary differential equation will be reduced to a first-order ordinary differential equation by this substitution. It can then be studied by the method of isoclinals.

The (x, y) plane is called the *phase plane*. This is natural, since x can be thought of as the *position*, while $y = \dot{x}$ can be thought of as the *velocity*, of a particle.

Let us consider, for a very simple example, the equation for a hramonic oscillator

$$\ddot{x} + \omega^2\,x = 0\,. \tag{6.14}$$

Using the redefinitions (6.11) and (6.12), the equation becomes

$$y\,\frac{dy}{dx} + \omega^2\,x = 0\,. \tag{6.15}$$

Proceeding now in the standard way, we see that the equation for the isoclinals is

$$y = -\frac{\omega^2\,x}{\lambda}\,, \tag{6.16}$$

and so they are straight lines of slope $-\omega^2/\lambda$ passing through the origin.

Of course in this toy example we can easily solve (6.15), giving

$$y^2 + \omega^2\,x^2 = c^2\,, \tag{6.17}$$

where c is an arbitrary constant. Thus the integral curves in the phase plane are ellipses, centred on the origin. Pretending, though, that we did not know this, we could discover the shape of these curves in the usual way by drawing curves in the phase plane whose slopes at the intersections with the isoclinals are given by λ. The isoclinals and integral curves are depicted in Figure 12 below.

The integral curves in Figure 12 show the relationship between the position x and the velocity $y = \dot{x}$ for the particle. Note that when $y = \dot{x}$ is positive, x must increase as t increases, and so it follows that the trajectory of the particle must be clockwise around the ellipse. The fact that the path closes on itself means that the motion of the particle is periodic. Of course in this toy example of the harmonic oscillator we already knew that, but in a more complicated equation it is useful to bear this in mind, as a way of recognising periodic motion.

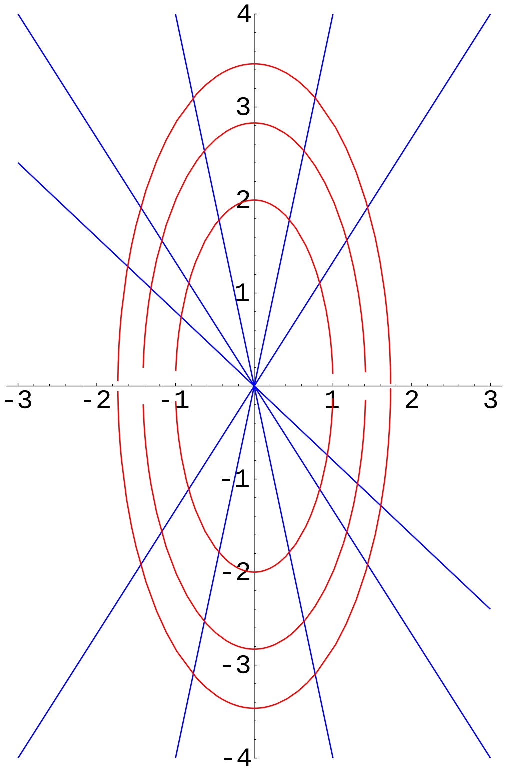

Figure 12: The isoclinal curves $y = -\omega^2\, x/\lambda$ (displayed in blue), and the integral curves (displayed in red) for the differential equation $y\, y' + \omega^2\, x = 0$. (Plotted for $\omega = 2$.)

Let us consider now a more complicated example, namely the van de Pol equation given in (6.10). This equation arises in certain physical situations where there is oscillatory motion that is not simple harmonic. After making the substitution $y = \dot{x}$, we obtain equation (6.13). For concreteness, let us take the constant ϵ to be $\epsilon = 1$. From (6.13), the equation for the isoclinals is

$$y = \frac{x}{1 - x^2 - \lambda}\,. \tag{6.18}$$

The phase-plane diagram for the van de Pol equation is depicted in Figure 13. As can be seen, the integral curves describe quite complicated paths in the phase plane, but in fact they all end up settling down to closed contours that go around the same track repeatedly, regardless of the initial conditions. Such closed tracks are called *limit cycles*. Thus the motion eventually becomes periodic, but it is not simple harmonic motion, which as we saw previously is characterised by elliptical contours in the phase plane.

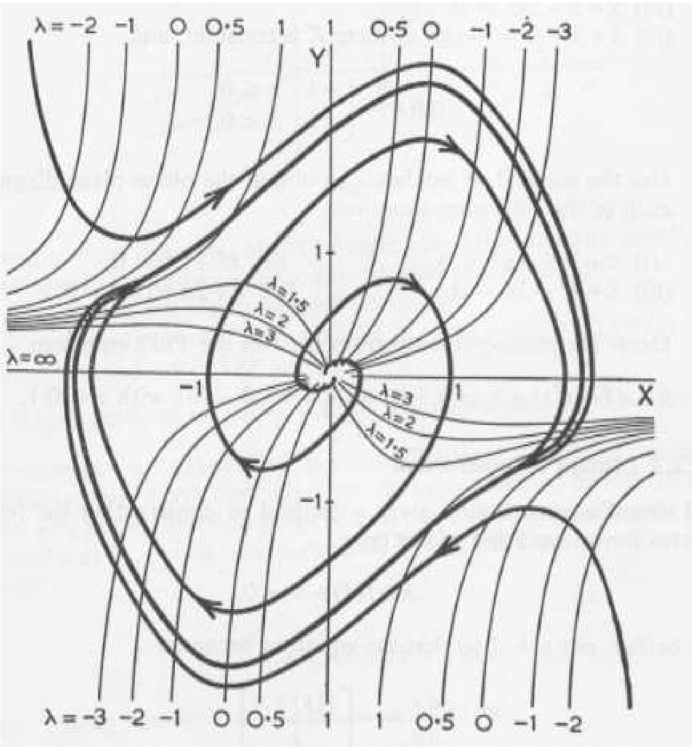

Figure 13: The phase-plane diagram for the van de Pol equation with $\epsilon = 1$. The light lines are the isoclinals, and the heavy lines are integral curves.

7 Cartesian Vectors and Tensors

7.1 Rotations and reflections of Cartesian coordinate

In Cartesian tensor analysis, one of the most fundamental notions is that of a *vector*. In an elementary introduction to vectors, the first example that one usually meets is the *position vector*, typically denoted by $\vec{r}$, which is thought of as the directed line connecting a point Q to another point P. In itself, this is a rather geometrical concept, which need not be linked to any specific choice of how the Cartesian coordinate system is chosen. For example, one could displace the origin of the coordinate system arbitrarily, and one could rotate the coordinate system arbitrarily. Of course often, one thinks of a position vector as a directed line from the *origin* O of the coordinate system to a given point P. In this case, the origin of the Cartesian coordinates would effectively be "pinned down," but the choice of how to orient the axes remains.

We commonly write the position vector $\vec{r}$ of a point P as a triple of numbers,

$$\vec{r} = (x, y, z)\,, \tag{7.1}$$

where x, y and z are nothing but the projections of the the line from O to P onto the x, y and z axes of the chosen system of Cartesian coordinates. The triple of numbers in (7.1) are called the *components* of the vector $\vec{r}$ with respect to this system of Cartesian coordinates. Of course, if we rotate to a new Cartesian coordinate system, then these three numbers will change. However, they will change in a specific and calculable way.

It is easier, for a simple illustration of what is going on, to think of the situation in 2, rather than 3, dimensions, so that a position vector is just specified by a pair of numbers,

$$\vec{r} = (x, y)\,, \tag{7.2}$$

these being the projections of the line OP onto the x and y axes of the chosen Cartesian coordinate system. Suppose now that we choose another Cartesian coordinate system, with the same origin O, but where the axes (x', y') are rotated anti-clockwise by an angle θ relative to the original axes (x, y). A simple application of trigononemtry shows that the components (x', y') of the position vector OP with respect to the new (or *primed*) coordinate system are related to its components (x, y) with respect to the original (or *unprimed*) coordinate system by

$$x' = x\,\cos\theta + y\,\sin\theta\,, \qquad y' = -x\,\sin\theta + y\,\cos\theta\,. \tag{7.3}$$

This can be written more elegantly as a matrix equation,

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}\,. \tag{7.4}$$

An essential property of the rotation described above is that the *length* of the vector $\vec{r}$, defined by

$$r \equiv |\vec{r}| = \sqrt{x^2 + y^2} \tag{7.5}$$

is the same whether we use the unprimed or the primed coordinate system. Namely, the rotation described by (7.3) or (7.4) has the property that

$$x'^2 + y'^2 = x^2 + y^2\,. \tag{7.6}$$

More generally, we can describe any rotation of the Cartesian coordinate system in a form analogous to (7.4), as

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = M \begin{pmatrix} x \\ y \end{pmatrix}\,. \tag{7.7}$$

where M is a 2×2 matrix that leaves the length of the vector $\vec{r}$ unchanged. Since we can write

$$x^2 + y^2 = (\, x\,, \quad y\,) \begin{pmatrix} x \\ y \end{pmatrix}\,, \tag{7.8}$$

it follows that the requirement (7.6) of preserving the length of the vector can be written as

$$(\, x\,, \quad y\,) \begin{pmatrix} x \\ y \end{pmatrix} = (\, x\,, \quad y\,)\; M^t\, M \begin{pmatrix} x \\ y \end{pmatrix}\,, \tag{7.9}$$

where M^t is the transpose of M. Since we want to require that the length of *any* vector $\vec{r}$ should be preserved, we can therefore strip off the (x, y) vectors in (7.9), and conclude that we must have

$$M^t\, M = \mathbb{1} \tag{7.10}$$

for any rotation, where $\mathbb{1}$ denotes the identity matrix. It is easily verified that for our rotation described in (7.4), the corresponding matrix

$$M = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \tag{7.11}$$

indeed satisfies (7.10).

Actually, the condition (7.10) allows for slightly more than just *rotations* of the Cartesian axes. It also allows for the possibility of making a *reflection* of the axes, such as

$$x' = x\,, \qquad y' = -y\,. \tag{7.12}$$

This would be described by the matrix

$$M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\,. \tag{7.13}$$

One can easily see that there is no choice of θ in (7.11) such that it becomes (7.13). Thus the full set of allowed length-preserving transformations of the Cartesian axes is composed of rotations together with reflections. In fact it is not hard to see that *any* arbitrary combination of rotation and reflection can be re-expressed as a rotation combined with a chosen *specific* reflection, such as the reflection about the x axis defined by (7.12). In other words, the full set of symmetry transformations that we can allow for our Cartesian coordinate systems comprises rotations about the origin, together with a possible reflection. The set of pure rotations, and the set of rotations plus reflections, are discretely different.

7.2 The orthogonal group $O(n)$, and vectors in n dimensions

In two dimensions it is easy enough to see all this explicitly, by writing down 2×2 matrices, but in higher dimensions it would be rather clumsy in general. It is therefore useful to abstract the essential features of the Cartesian coordinate rotations and reflection, in a fashion that can expressed succinctly in any dimension. First of all, in n dimensions it is convenient to label our Cartesian axes by $(x_1, x_2, \ldots, x_n)$, so that we don't run out of letters of the alphabet. We can then describe the allowed transformations of the Cartesian coordinates by

$$\begin{pmatrix} x_1' \\ x_2' \\ \vdots \\ x_n' \end{pmatrix} = M \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \tag{7.14}$$

where in order to preserve the length, the $n\times n$ matrix M must satisfy

$$M^t\, M = 1\!\!1\,. \tag{7.15}$$

Such $n\times n$ matrices satisfying (7.15) are called *orthogonal* matrices, and this is denoted by $O(n)$. This terminology is derived from group theory, and signifies that the set of all $n\times n$ matrices satisfying (7.15) form a group. For any pair of $O(n)$ matrices M_1 and M_2 the matrix product

$$M_3 \equiv M_1\, M_2 \tag{7.16}$$

is another $O(n)$ matrix. The full set of requirements for a group are:

1 There must be an *associative* law of combination for all group elements a, b and c, such that $a\cdot(b\cdot c) = (a\cdot b)\cdot c$.

2 For any group elements a and b, the combination $a\cdot b$ must be a group element too.

3 There must exist an *identity element* e, such that $a\cdot e = e\cdot a = a$ for any group element a.

4 Every group element a must have an inverse, a^{-1}, such that $a^{-1}\cdot a = a\cdot a^{-1} = e$.

For our case, the law of combination is simply the multiplication of matrices. Obviously this is associative, so requirement 1 is satisfied. As already noted, requirement 2 is satisfied too, since we shall have

$$\begin{aligned} M_3^t\, M_3 &= (M_1\, M_2)^t\, M_1\, M_2 = M_2^t\, M_1^t\, M_1\, M_2\,, \\ &= M_2^t\, 1\!\!1\, M_2 = M_2^t\, M_2 = 1\!\!1\,. \end{aligned} \tag{7.17}$$

Requirement 3 is clearly satisfied, and we simply have that $e = \mathbb{1}$, the identity matrix. Finally, we can see straight away from (7.15) that in this case the inverse of M is nothing but

$$M^{-1} = M^t \,. \tag{7.18}$$

We can also see easily how to characterise the cases where the transformation includes a reflection as well as a rotation. From (7.15), we can take the determinant, and using elementary properties we find

$$\begin{aligned} \det(M^t\, M) &= \det(M^t)\, \det(M) = (\det M)^2 \,, \\ &= \det \mathbb{1} = 1 \,. \end{aligned} \tag{7.19}$$

Thus we deduce that $O(n)$ matrices satisfy

$$\det M = \pm 1 \,. \tag{7.20}$$

We give the name $SO(n)$ to $O(n)$ matrices whose determinant is $+1$, the "S" standing for "special." Clearly the product of any two $SO(n)$ matrices is also in $SO(n)$,

$$\det(M_1\, M_2) = (\det M_1)\, (\det M_2) = 1 \,, \tag{7.21}$$

and so $SO(n)$ is a *subgroup* of $O(n)$. The group of $SO(n)$ matrices describes the situation of *pure rotations.* If an $O(n)$ matrix M is such that $\det M = -1$, then it must be that M describes a *rotation* plus a *reflection.* Note that the set of all $\det M = -1$ matrices *do not* form a group, since the product of two such matrices will have determinant $+1$.

It is easy to see that a $\det M = -1$ transformation necessarily includes a reflection, by looking at examples. It is also clear from the fact that $\det M = +1$ matrices can be continuously connected to the identity, whilst $\det M = -1$ matrices involve a discrete transition from the identity. For example, in (7.11) we can continuously increase θ from 0 to its final value. By contrast, since $\det \mathbb{1} = +1$ but the determinant of the matrix in (7.13) is -1, it is obvious that we cannot perform a continuous sequence of deformations of $\mathbb{1}$ into the matrix in (7.13).

7.3 Cartesian vectors and tensors

Now let us continue with the main theme, of Cartesian vector and tensor analysis. We may take the position vector as the prototype of all vectors, and thus we may define a vector V in n dimensions[30] by saying that it has components $(V_1, V_2, \ldots V_n)$ that transform under rotations of the Cartesian frame in a manner identical to that for the position vector, namely

$$\begin{pmatrix} V_1' \\ V_2' \\ \vdots \\ V_n' \end{pmatrix} = M \begin{pmatrix} V_1 \\ V_2 \\ \vdots \\ V_n \end{pmatrix} . \qquad (7.22)$$

It is very convenient at this stage to introduce an index notation, so that we don't have to write out big n-component column vectors. Thus we label the rows and columns of the $n \times n$ matrix M by indices i and j, so that

$$M = \begin{pmatrix} M_{11} & M_{12} & \cdots & M_{1n} \\ M_{21} & M_{22} & \cdots & M_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ M_{n1} & M_{n2} & \cdots & M_{nn} \end{pmatrix} . \qquad (7.23)$$

The equation (7.22) can then be written as

$$V_i' = \sum_{j=1}^{n} M_{ij}\, V_j \,. \qquad (7.24)$$

A further hugely simplifying refinement, introduced by Einstein, is to recognise that in any valid vector or tensor expression, a summation symbol will always be needed when a particular index occurs exactly twice in an expression, such as the j index in (7.24). Furthmore, there will never be any circumstance in a valid expression when an index occurs twice without the need for the summation. Therefore, in the *Einstein Summation Convention*, we may simply write (7.24) as

$$V_i' = M_{ij}\, V_j \,, \qquad (7.25)$$

with the repetition of the "dummy suffix" j meaning that a summation over its index-range (1 to n) is understood.

Notice that the orthogonality condition (7.15) satisfied by the matrix M can also be written simply in terms of the index notation. First, note that if A and B are matrices, with components A_{ij} and B_{ij} respectively, then the matrix $C \equiv A\, B$ will have components given by

$$C_{ij} = A_{ik}\, B_{kj} \,. \qquad (7.26)$$

[30]It is customary, at least in the USA, to use the arrow symbol to denote a vector in three dimensions, thus $\vec{V}$. In a general dimension n, it is more tradiational not to use an arrow, but simply to denote the vector by V. We shall follow the tradition.

The multiplication with the summation over k precisely corresponds to the matrix operation of multiplying the rows of A into the columns of B. Next, we note that the process of transposing a matrix means precisely that we exchange the roles of the rows and the columns, which means that the components of the transpose of M are given by

$$(M^t)_{ij} = M_{ji}\,. \tag{7.27}$$

Finally, we note that the components of the unit matrix are nothing but δ_{ij}, the Kronecker delta, which is zero if $i \neq j$ and 1 if $i = j$. Therefore (7.15) is written as

$$(M^t)_{ik}\, M_{kj} = \delta_{ij}\,, \tag{7.28}$$

and hence we have

$$M_{ki}\, M_{kj} = \delta_{ij}\,. \tag{7.29}$$

Suppose now that we have two vectors U and V. This means that we know that under a rotation[31] of the Cartesian coordinates, their components U_i and V_i will transform as

$$U_i' = M_{ij}\, U_j\,, \qquad V_i' = M_{ij}\, V_j\,. \tag{7.30}$$

We may now define the notion of the *inner product*, or *dot product* of U and V. Let us call this quantity f. We can define this in terms of the components, as

$$f \equiv U_i\, V_i\,. \tag{7.31}$$

We can now easily see that f is a *scalar*, which means that it is completely invariant under rotations of the coordinate system. We prove this by using the transformation rules for U and V given in (7.30), which allows us to calculate what the quantity f' defined by (7.31), but for the primed components, in terms of f itself:

$$\begin{aligned} f' &\equiv U_i'\, V_i' \\ &= M_{ij}\, U_j\, M_{ik}\, V_k \\ &= \delta_{jk}\, U_j\, V_k \\ &= U_j\, V_j \\ &= f\,. \end{aligned} \tag{7.32}$$

[31]We will sometimes loosely use the word "rotation," as a shorthand for "rotation or rotation and reflection." On occasions when it is important to be precise about whether reflections are included, we will emphasise the point specifically.

Thus $f' = f$, proving that f is a scalar under coordinate rotations. Note that a special case of an inner product is when one takes the inner product of a vector with itself, as

$$f = V_i\, V_i\,. \tag{7.33}$$

A moment's thought will convince the reader that $V_i\, V_i$ is nothing but the norm-squared of the vector V, and more generally $U_i\, V_i$ is nothing but the usual dot product or scalar product of the vectors U and V.

We have now met scalars, which are invariant under coordinate rotations, and vectors, whose components rotate in the specific way (7.25). It is not a big extension of these notions to enlarge the discussion to quantities with more than one index. These are called *tensors*. To be precise, a p-index quantity $T_{i_1\cdots i_p}$ is a tensor under coordinate rotations if it transforms in the following very specific way:

$$T'_{i_1\cdots i_p} = M_{i_1 j_1}\, M_{i_2 j_2} \cdots M_{i_p j_p}\, T_{j_1\cdots j_p}\,. \tag{7.34}$$

Thus each index simultaneously transforms with a rotation matrix M. This tensor T is called a rank-p tensor.

It is obvious from the (7.25) that if we define the so-called *outer product* of two vectors U and V, as the quantity T with components

$$T_{ij} = U_i\, V_j\,, \tag{7.35}$$

then this transforms precisely as a rank-2 tensor:

$$T'_{ij} = M_{ik}\, M_{j\ell}\, T_{k\ell}\,. \tag{7.36}$$

Obviously one can make higher-rank tensors by taking outer products of larger numbers of vectors. Not all tensors, hwoever, are simply the outer products of vectors. More generally, a tensor can be expressed as the *sum* of a number of outer products of vectors. One can also, of course, take outer products of tensors to make bigger tensors of higher rank.

It is very easy to see that if one *contracts* a pair of indices on a tensor of rank p, then one gets a tensor of rank $p-2$. The process of contacting indices means setting two of them equal. Then, the Einstein summation convention comes into play, meaning that we have the understanding that the two indices are then summed over. For example, suppose we have a rank-3 tensor T_{ijk}. We can make a rank-1 tensor (i.e. a vector) by contracting a pair of indices, for example we can define

$$V_i \equiv T_{ijj}\,. \tag{7.37}$$

The proof that V_i really is a vector is the usual one; namely, to show that it really does transform like a vector under coordinate rotations. We do this by starting from the known transformation rule of T_{ijk}, which by definition, since we are told that it is a tensor, transforms as

$$T'_{ijk} = M_{i\ell}\, M_{jm}\, M_{kn}\, T_{\ell mn}\,. \tag{7.38}$$

Notice by the way, that we must always be very careful not to abuse the Einstein summation convention. If there are multiple dummy indices to be summed over, as with ℓ, m and n here, then we must make sure that we have invented a new dummy suffix name for each separate summation. Thus, for example, if we tried writing the right-hand side of (7.38) as

$$M_{i\ell}\, M_{jm}\, M_{km}\, T_{\ell mm}\,, \tag{7.39}$$

then this would be complete nonsense, since we have the dummy suffix m occuring 4 times, and we wouldn't know which pairs were supposed to be summed over. It would be like writing a computer program with multiple summation labels in a multiple sum, and then inadvertently using the same index label for two summations that were meant to be distinct.

Going back to our example, we now check that V_i transforms properly as a vector by its definition (7.37), but now expressed for the primed coordinate frame, and then applying the known transformation rule (7.38) for T_{ijk}. Thus we get

$$\begin{aligned} V'_i &\equiv T'_{ijj} \\ &= M_{ik}\, M_{j\ell}\, M_{jm}\, T_{k\ell m} \\ &= M_{ik}\, \delta_{\ell m}\, T_{k\ell m} \\ &= M_{ik}\, T_{k\ell\ell} \\ &= M_{ik}\, V_k\,, \end{aligned} \tag{7.40}$$

and so indeed it transforms in the way a vector should.

In general, any operation of taking outer products, inner products, or contractions will cause a tensorial expression to turn into another tensorial expression with more, or less, indices as the case may be. A nice thing about it is that after getting accustomed to the formalism, one doesn't need to check every time whether an expression made from tensors is itself a tensor. As long as only valid procedures are used, such as taking outer or inner products or contractions, the bottom line is that "if it looks like a tensor, it is a tensor."

7.4 Invariant tensors, and the cross product

We have seen that in general the components of a tensor transform in a non-trivial way under rotations of the Cartesian coordinate system. There are certain exceptional tensors, however, which have the property that their components do not transform at all under rotations. Such tensors are called *Invariant Tensors*.

7.4.1 The Kronecker delta tensor

We have in fact already met one example, namely the Kronecker delta symbol δ_{ij}. Recalling the defining property (7.15) for $O(n)$ matrices M, we may first note that $M^t\, M = \mathbb{1}$ implies also $M\, M^t = \mathbb{1}$, for we have

$$M\, M^t\, M = M\,, \tag{7.41}$$

and hence

$$M\, M^t = M\, M^{-1} = \mathbb{1}\,. \tag{7.42}$$

Thus as well as (7.29), we also have that if M is an $O(n)$ matrix then it satsifies

$$M_{ik}\, M_{jk} = \delta_{ij}\,. \tag{7.43}$$

This can be written as

$$\delta_{ij} = M_{ik}\, M_{j\ell}\, \delta_{k\ell}\,. \tag{7.44}$$

Comparing with the general tensor transformation rule (7.34), we therefore see that the Kronecker delta δ_{ij} is an invariant tensor, in the sense that if we define it to have the same structure in any Cartesian coordinate system, namely that it vanishes if $i \neq j$ and equals 1 if $i = j$, then it obeys the usual tensor transformation rule, but with the special property that its components are completely unaltered under arbitrary rotations:

$$\delta'_{ij} = \delta_{ij}\,. \tag{7.45}$$

Note that immediate properties of the Kronecjker delta tensor are

$$\delta_{ij}\, \delta_{jk} = \delta_{ik}\,, \qquad \delta_{ii} = n\,. \tag{7.46}$$

(The summation over repeated indices is understood, as usual. In the second expression, δ_{ii} is therefore the trace of the identity matrix in n dimensions; hence the result n.)

Note that the Kronecker delta tensor can be viewed as the basic building block of the scalar product of two vectors A and B:

$$A \cdot B = A_i\, B_j\, \delta_{ij} = A_i\, B_i\,. \tag{7.47}$$

Of course, given δ_{ij} one can trivially construct lots of other invariant tensors, by taking outer products of Kronecker deltas. For example

$$T_{ijk\ell} \equiv \delta_{ij}\, \delta_{k\ell} \tag{7.48}$$

is a rank-4 invariant tensor. There is, however, one further invariant tensor that can be written down, which is not merely constructed from products of Kronecker deltas. This tensor, denoted by $\varepsilon_{i_1\cdots i_n}$ in n dimensions, is sometimes called the Levi-Civita tensor.

7.4.2 The Levi-Civita (pseudo) Tensor

In n dimensions, the Levi-Civita tensor (or pseudo-tensor, as we should more properly call it; see later) has n indices. It is defined by the following rules. Firstly, it is *totally antisymmetric* in all n of its indices, which means that if any pair of indices is exchanged, it changes sign:

$$\varepsilon_{i_1 i_2\cdots i_n} = -\varepsilon_{i_2 i_1\cdots i_n}\,, \tag{7.49}$$

and similarly for *any* exchange of two indices. Finally, we specify that

$$\varepsilon_{123\cdots n} = +1\,. \tag{7.50}$$

This is enough to specify it completely. By the antisymmetry rule, any *even* permutation of the indices $1, 2, \ldots, n$ will give $+1$, while any *odd* permutation of the indices $1, 2, \ldots, n$ will give -1. If any two indices on $\varepsilon_{i_1\cdots i_n}$ are equal, then the antisymmetry property implies that it will vanish. Thus all the cases have been covered.

To see that $\varepsilon_{i_1\cdots i_n}$ is an invariant tensor under rotations[32], we need a result from matrix theory. The relevant fact is that if A is any $n\times n$ matrix with components A_{ij}, then

$$A_{i_1 j_1}\, A_{i_2 j_2} \cdots A_{i_n j_n}\, \varepsilon_{j_1 j_2\cdots j_n} = (\det A)\, \varepsilon_{i_1 i_2\cdots i_n}\,. \tag{7.51}$$

After some thought it is not hard to see that this is true. It is helpful to play around with a simple example such as $n = 2$. In two dimensions, the statement is that

$$A_{ik}\, A_{j\ell}\, \varepsilon_{k\ell} = (\det A)\, \varepsilon_{k\ell}\,. \tag{7.52}$$

Bearing in mind that we have $\varepsilon_{12} = -\varepsilon_{21} = 1$, $\varepsilon_{11} = \varepsilon_{22} = 0$, we can then consider the possible cases for the free indices i and j in (7.52). For example, with $i = 1$, $j = 2$ we find that the left-hand side gives

$$A_{11}\, A_{22} - A_{12}\, A_{21}\,, \tag{7.53}$$

[32] Here, as we shall see below, we must be precise, and emphasise that this statement is true only for pure rotations, but not rotations with reflections.

which indeed agrees with the right-hand side, which is $\det A$ times ε_{12}, or in other words $\det A$. With $i=1$, $j=1$, on the other hand, one gets $0=0$. In a similar fashion, all the other components are consistent with (7.52).

In an arbitrary dimension, it is easy to see that unless the free indices $i_1 \cdots i_n$ in (7.51) are taken to be $1 \cdots n$, or some permutation thereof, both sides of the equation will be zero. Since there is manifest total antisymmetry on both sides of equation (7.51), it suffices to check just one of the $n!$ possible non-zero cases, which for simplicity we can take to be $i_1 - 1$, $i_2 = 2, \ldots, i_n = n$. It is rather straightforward to see that the left-hand side is in fact constructing the determinant for us. Let us agree to believe, then, that (7.51) is true in arbitrary dimensions.

We now apply (7.51) to the case of an $SO(n)$ matrix M. It will be recalled that this has the property $\det M = +1$, and it describes a pure rotation of Cartesian coordinates, with no reflection. We therefore have

$$\varepsilon_{i_1 i_2 \cdots i_n} = M_{i_1 j_1}\, M_{i_2 j_2} \cdots M_{i_n j_n}\, \varepsilon_{j_1 j_2 \cdots j_n}\,. \tag{7.54}$$

Comparing with (7.34), we see that $\varepsilon_{i_1 i_2 \cdots i_n}$ obeys the general rule for the transformation of a tensor under coordinate rotations, but with the special property that

$$\varepsilon'_{i_1 i_2 \cdots i_n} = \varepsilon_{i_1 i_2 \cdots i_n}\,. \tag{7.55}$$

Just like δ_{ij}, therefore, $\varepsilon_{i_1 i_2 \cdots i_n}$ is an *invariant* tensor under rotations. However, there is a subtlety here. The Kronecker delta is also a tensor under *reflections* as well as pure rotations. By contrast, $\varepsilon_{i_1 i_2 \cdots i_n}$ is not. As we see from (7.51), for an arbitrary rotation together, possibly, with rotations, we must write

$$\varepsilon_{i_1 i_2 \cdots i_n} = M_{i_1 j_1}\, M_{i_2 j_2} \cdots M_{i_n j_n}\, (\det M)\, \varepsilon_{j_1 j_2 \cdots j_n} \tag{7.56}$$

instead of (7.54). If we include the reflections, then the set of quantities $\varepsilon_{i_1 i_2 \cdots i_n}$ defined by total antisymmetry and $\varepsilon_{12 \cdots n} = 1$ in all frames does not transform like a normal tensor, but instead it picks up a minus sign if a reflection is involved. Quantities that transform like tensors under pure rotations, but with an extra minus sign under reflections, are called *pseudo-tensors*. Often, if one is just speaking "casually," one tends to refer to them simply as tensors.

The Levi-Civita pseudo-tensor plays an important role in vector and tensor analysis. A very important property concerns the product of two Levi-Civita pseudo-tensors. It is probably easiest to describe this by starting with low-dimensional examples. In two dimensions, we have ε_{ij}, with $\varepsilon_{12} = -\varepsilon_{21} = 1$, $\varepsilon_{11} = \varepsilon_{22} = 0$. It is easy to see, simply by checking all the possible index assignments, that

$$\varepsilon_{ij}\,\varepsilon_{k\ell} = \delta_{ik}\,\delta_{j\ell} - \delta_{i\ell}\,\delta_{jk}\,. \tag{7.57}$$

(Try it for a few choices, such as $i = 1$, $j = 2$, $k = 1$, $\ell = 2$, etc.)

In three dimensions, the analogous product rule involves 6 terms rather than 2 on the right-hand-side:

$$\varepsilon_{ijk}\,\varepsilon_{\ell mn} = \delta_{i\ell}\,\delta_{jm}\,\delta_{kn} + \delta_{in}\,\delta_{j\ell}\,\delta_{km} + \delta_{im}\,\delta_{jn}\,\delta_{k\ell} - \delta_{i\ell}\,\delta_{jn}\,\delta_{km} - \delta_{im}\,\delta_{j\ell}\,\delta_{kn} - \delta_{in}\,\delta_{jm}\,\delta_{k\ell}\,. \tag{7.58}$$

Looking at this, one can see the pattern. The first term on the right-hand side has the product of a Kronecker delta linking the first indices on the two epsilon tensors, a Kronecker delta linking the second indices on the two epsilon tensors, and a Kronecker delta linking the last indices on the two epsilon tensors. Then, there are 5 more terms, which correspond to permuting around the ℓ, m and n indices, with a plus sign for an even permutation, and a minus sign for an odd permutation. There are in total 3! possible permutations, hence the six terms on the right-hand side. The need for this permutation antisymmetry in the expression on the right-hand side is obvious, since we know that it is an antisymmetry of the left-hand side. Note also that although as stated above, the implementation of the permutation antisymmetry of ℓ, m and n might seem to have been favoured over the permutation antisymmetry of i, j, k, in fact everything is perfectly democratic. Having enforced the antisymmetry in ℓ, m and n on the right-hand side, it implies (as can easily be seen by inspection) an antisymmetry in i, j and k as well.

It is not hard to prove (7.58), again by looking at all the possible index assignments for i, j, k, ℓ, m and n. This is not as daunting a task as it might sound, because of the antisymmetries discussed above. In fact, if one thinks about it, there are very few cases that need to be checked explicitly; the rest all follow by invoking the permutation symmetries.

The general expression for the product of two epsilon tensors in n dimensions will involve $n!$ sums of products of Kronecker deltas on the right-hand side:

$$\varepsilon_{i_1\cdots i_n}\,\varepsilon_{j_1\cdots j_n} = \delta_{i_1 j_1}\cdots\delta_{i_n j_n} + \text{even perms} - \text{odd perms}\,. \tag{7.59}$$

7.4.3 Three-dimensional vector identities

A very useful consequence of (7.58) in 3 dimensions arises if we set $k = n$ (which means, of course, that this repeated index is then summed over 1, 2 and 3.) Bearing in mind the properties of the Kronecker delta, given in (7.46), we therefore find (after a convenient relabelling of indices)

$$\varepsilon_{ijm}\,\varepsilon_{k\ell m} = \delta_{ik}\,\delta_{j\ell} - \delta_{i\ell}\,\delta_{jk}\,. \tag{7.60}$$

This identity allows us to derive very easily some of the basic Cartesian vector identities in three dimensions.

First, we note that the *vector product* $\vec{A}\times\vec{B}$ of vectors $\vec{A}$ and $\vec{B}$ gives a quantity $\vec{C}\equiv\vec{A}\times\vec{B}$ whose components are given by

$$\vec{C} = (C_1, C_2, C_3) = (A_2\,B_3 - A_3\,B_2, A_3\,B_1 - A_1\,B_3, A_1\,B_2 - A_2\,B_1)\,, \tag{7.61}$$

which can be written very succinctly using the epsilon pseudo-tensor, as

$$C_i = (\vec{A}\times\vec{B})_i = \varepsilon_{ijk}\,A_j\,B_k\,. \tag{7.62}$$

It is straightforward to show, by the standard procedure of calculating the components C_i' in a transformed Cartesian coordinate system, that $\vec{C}$ transforms like a vector under pure rotations, but it acquires an extra (-1) factor under rotations with a reflection, owing to the $\det M$ factor in the transformation rule for ε_{ijk}. Therefore $\vec{C}$ is a pseudo-vector. One immediately sees the antisymmetry of the vector product, $\vec{A}\times\vec{B} = -\vec{B}\times\vec{A}$, from the antisymmetry of ε_{ijk}.

Some vector identities now follow very straightforwardly. First, we may note that for any set of three 3-vectors $\vec{A}$, $\vec{B}$ and $\vec{C}$, the scalar quantity known as their *scalar triple product*, $\vec{A}\cdot(\vec{B}\times\vec{C})$, can be written using ε_{ijk} as

$$\vec{A}\cdot(\vec{B}\times\vec{C}) = \varepsilon_{ijk}\,A_i\,B_j\,C_k\,. \tag{7.63}$$

It is now immediately obvious, from the total antisymmetry of ε_{ijk}, that (7.63) is totally antisymmetric under any exchange of the vectors. Thus, we have

$$\begin{aligned}\vec{A}\cdot(\vec{B}\times\vec{C}) &= \vec{B}\cdot(\vec{C}\times\vec{A}) = \vec{C}\cdot(\vec{A}\times\vec{B})\\ &= -\vec{A}\cdot(\vec{C}\times\vec{B}) = -\vec{B}\cdot(\vec{A}\times\vec{C}) = -\vec{C}\cdot(\vec{B}\times\vec{A})\,.\end{aligned} \tag{7.64}$$

A special case following from the above is, of course, that $\vec{A}\cdot(\vec{A}\cdot\vec{B}) = 0$.

Of course, strictly speaking $\vec{A}\cdot(\vec{B}\times\vec{C})$ is not an scalar, but a pseudo-scalar, since it is constructed using the epsilon pseudo-tensor. Thus unlike an ordinary scalar, which is invariant both under rotations *and* reflections, $\vec{A}\cdot(\vec{B}\times\vec{C})$ is invariant under pure rotations, but it changes sign under reflections.

Now, let us consider the *vector triple product* of any three 3-vectors $\vec{A}$. $\vec{B}$ and $\vec{C}$. This is defined as the vector $\vec{D}$, given by

$$\vec{D} = \vec{A} \times (\vec{B} \times \vec{C})\,. \tag{7.65}$$

From (7.62), we see that we can write the components of $\vec{D}$ as

$$D_i = \varepsilon_{ijm}\, \varepsilon_{mk\ell}\, A_j\, B_k\, C_\ell\,. \tag{7.66}$$

Note that $\vec{D}$ is an ordinary vector, and not a pseudo-vector. This is because it involves *two* epsilon pseudo-tensors in its definition (7.66) in terms of the vectors $\vec{A}$, $\vec{B}$ and $\vec{C}$, and so the two $\det M$ factors that will arise when checking the transformation rule for $\vec{D}$ will multiply and give $(+1)$, even under reflections.

The fact that $\vec{D}$ is a true vector is also evident from (7.60), which shows that the product of the two epsilon pseudo-tensors can be re-expressed in terms of products of Kronecker delta tensors. In fact using (7.60), we can re-express (7.65) in terms of scalar products. First, it is worth noting that because ε_{ijk} has an *odd* number of indices, any rearrangement of the indices that is achieved by a *cyclic* permutation implies an *even* number of index-pair exchanges, and so it leaves the sign of the epsilon tensor unchanged. In other words

$$\varepsilon_{ijk} = \varepsilon_{jki} = \varepsilon_{kij}\,. \tag{7.67}$$

Therefore, it follows that we can cycle $\varepsilon_{mk\ell}$ to $\varepsilon_{k\ell m}$ in (7.66) with no sign change, and then, using (7.60), we get

$$D_i = (\delta_{ik}\, \delta_{j\ell} - \delta_{i\ell}\, \delta_{jk})\, A_j\, B_k\, C_\ell\,. \tag{7.68}$$

Using the index-replacement rules for the Kronecker delta tensor, this implies

$$D_i = B_i\, A_j\, C_j - C_i\, A_j\, B_j\,. \tag{7.69}$$

Thus, writing it back in 3-vector notation, we have

$$\vec{D} \equiv \vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}\,(\vec{A}\cdot\vec{C}) - \vec{C}\,(\vec{A}\cdot\vec{B})\,. \tag{7.70}$$

There are many other examples of vector expressions that can be simplified using the basic identities (7.60), or (7.58) for the epsilon tensor. The rule is that whenever an expression involves two or more vector product symbols "×", then they can be eliminated pairwise, being replaced by scalar products. Once one is familiar with the basic structure of (7.60), most expressions capable of such simplifications can be handled. It is so simple to derive the results "as needed" that it is no longer worth taking the trouble to remember a formula such as (7.70); it is easier to derive it as and when needed. Memorising (7.60) is itself very simple; with the contracted index being "3'rd with 3'rd" on the epsilon tensors, the right-hand side is the product of "1'st with 1'st" and "2'nd with 2'nd" Kronecker deltas, minus "1'st with 2'nd" and "2'nd with 1'st."

7.4.4 Hodge dualisation

The notation in three-dimensional Cartesian vector analysis of constructing a vector $\vec{C}$ from the vector product $\vec{C} \equiv \vec{A} \times \vec{B}$ of two vectors $\vec{A}$ and $\vec{B}$ is such a commonplace that it sometimes surprises people to learn that it works only in three dimensions. The crucial quantity involved in the construction of the vector product is the 3-index epsilon tensor ε_{ijk}, and it has three indices precisely because of being in three dimensions.

The notation that *does* generalise to an arbitrary dimension is that from any pair of vectors A and B we can form an antisymmetric rank-2 tensor W whose components W_{ij} are defined by

$$W_{ij} = A_i\, B_j - A_j\, B_i\,. \tag{7.71}$$

In three dimensions, we can map back and forth between W_{ij} and the vector C_i defined above, by making use of the 3-index epsilon tensor:

$$\begin{aligned} C_i &= \tfrac{1}{2}\varepsilon_{ijk}\, W_{jk} = \varepsilon_{ijk}\, A_j\, B_k\,, \\ W_{ij} &= \varepsilon_{ijk}\, C_k\,. \end{aligned} \tag{7.72}$$

Note that this ability to map *both ways* can be seen using (7.60). Thus, given $C_i = \frac{1}{2}\varepsilon_{ijk}\, W_{jk}$, we calculate

$$\varepsilon_{ijk}\, C_k = \tfrac{1}{2}\varepsilon_{ijk}\, \varepsilon_{k\ell m}\, W_{\ell m} = \tfrac{1}{2}(\delta_{i\ell}\, \delta_{jm} - \delta_{im}\, \delta_{j\ell})\, W_{\ell m} = W_{ij}\,. \tag{7.73}$$

So in three dimensions, having a 2-index antisymmetric tensor is essentially equivalent to having a vector, since we can map freely backwards and forwards. (It is essential, of course, that W_{ij} itself be *antisymmetric* in order for this invertible mapping to work.)

In higher dimensions, the nature of the mapping is different. For example, in four dimensions we have a 4-index epsilon tensor, and so from W_{ij} we can make another 2-index antisymmetric tensor:

$$Z_{ij} \equiv \varepsilon_{ijk\ell}\, W_{k\ell}\,. \tag{7.74}$$

This is again invertible, and in fact from (7.59) one can prove that

$$W_{ij} = \tfrac{1}{4}\varepsilon_{ijk\ell}\, Z_{k\ell}\,. \tag{7.75}$$

It is not so immediately obvious in four dimensions what the point of mapping from one 2-index antisymmetric tensor into the other would be, since one has not achieved any reduction of the number of indices. Actually, it turns out that there are important uses for this procedure, and in fact a special significance is attached to 2-index tensors that have the property of mapping into themselves under this transformation.

The mapping process is known as *Hodge Dualisation*. To make the combinatorics work nicely, it is better to put in a factorial coefficient. The Hodge dual of a rank-2 antisymmetric tensor W_{ij} in four dimensions is denoted by W^*_{ij}, and defined by

$$W^*_{ij} = \frac{1}{2!}\varepsilon_{ijk\ell}\, W_{k\ell}\,. \tag{7.76}$$

From this, one can show using (7.59) that

$$W_{ij} = \frac{1}{2!}\varepsilon_{ijk\ell}\, W^*_{k\ell}\,. \tag{7.77}$$

If a tensor happens to satisfy $W_{ij} = \pm W^*_{ij}$, it is called self-dual or anti-self-dual respectively.

More generally, if we are in n dimensions and we have a rank-p antisymmetric tensor $T_{i_1\cdots i_p}$, then its Hodge dual is a rank-$(n-p)$ tensor with components $T^*_{i_1\cdots i_{n-p}}$ given by

$$T^*_{i_1\cdots i_{n-p}} \equiv \frac{1}{p!}\,\varepsilon_{i_1\cdots i_{n-p}j_1\cdots j_p}\, T_{j_1\cdots j_p}\,. \tag{7.78}$$

The procedure of making a vector $\vec C = \vec A\times\vec B$ out of two vectors $\vec A$ and $\vec B$ in three dimensions can now be understood as a special case, in which one takes the Hodge dual of the 2-index antisymmetric tensor with components $A_i\, B_j - A_j\, B_i$.

Notice, by the way, that one of our familiar concepts in three dimensions is that rotations occur *around axes*. This is a very special feature of three dimensions, for precisely the reasons we have been discussing. Think of the angular momentum vector,

$$\vec L = \vec r\times\vec p\,, \tag{7.79}$$

for example, which, in components, would be written

$$L_i = \varepsilon_{ijk}\, x_j\, p_k\,. \tag{7.80}$$

In a general dimension, we would instead simply view the angular momentum as a 2-index antisymmetric tensor,

$$L_{ij} = x_i\, p_j - x_j\, p_i\,. \tag{7.81}$$

Thus in a general dimension, a rotation occurs *in a 2-plane*, which is specified as the plane in which the position vector $\vec r$ and the linear momentum vector $\vec p$ lie. It is a "coincidence" of living in three spatial dimensions that instead of saying "a rotation in the (x,y) plane," we can say "a rotation around the z axis."

7.5 Cartesian Tensor Calculus

The basic differential operator in vector and tensor calculus is the gradient operator ∇. This is the vector-valued operator whose "components" are the set of partial derivatives with respect to the Cartesian coordinates x_i. For brevity, let us define

$$\partial_i \equiv \frac{\partial}{\partial x_i} \,. \tag{7.82}$$

Then we shall have

$$\vec{\nabla} = (\partial_1, \partial_2, \ldots, \partial_n) \tag{7.83}$$

in n dimensions.

We can easily see that ∇ is indeed a vector; the proof is the usual one, of showing that its components transform as a vector under rotations of the Cartesian coordinates. Thus in a rotated coordinate system x_i', for which, *by definition*, we have $\partial_i' = \partial/\partial x_i'$, we find, using the chain rule,

$$\partial_i' = \frac{\partial x_j}{\partial x_i'}\, \partial_j \,. \tag{7.84}$$

Now we have $x_i' = M_{ij}\, x_j$ under the coordinate rotations, and so, multiplying by M_{ik} and using (7.29), we have $M_{ik}\, x_i' = x_k$. Differentiating (take care of the index choices!) we find $\frac{\partial x_j}{\partial x_i'} = M_{ij}$, and so we conclude that

$$\partial_i' = M_{ij}\, \partial_j \,. \tag{7.85}$$

This proves that ∂_i transforms exactly as a vector should, under rotations of the Cartesian axes.

It is now straightforward to see that if ∇ acts on any scalar field ϕ, it will give a vector, $\nabla\phi$. In fact more generally, if ∇ acts on any rank-p tensor T, it will give a rank-$(p+1)$ tensor S, with components given by

$$S_{ij_1\cdots j_p} = \partial_i\, T_{j_1\cdots j_p} \,. \tag{7.86}$$

The proof is the usual one, of showing that $S_{ij_1\cdots j_p}$ transforms with the proper tensor transformation law (7.34) under rotations of the Cartesian coordinates. Of course, having established that $\partial_i\, T_{j_1\cdots j_p}$ is a tensor, all the usual rules follow. In particular, for example, it follows that we can take a *divergence* of the tensor $T_{j_1\cdots j_p}$, by contracting the index i on the derivative in (7.86) with one of the indices on $T_{j_1\cdots j_p}$, and thereby get a rank-$(p-1)$ tensor. (In general, if $T_{j_1\cdots j_p}$ has no special symmetry properties on its indices, there will be p different divergences that we can make, depending on which of the j indices we choose to contract with the i index.)

A special case of the above is to form the scalar quantity $\partial_i V_i$ as the divergence of the vector V_i.

Note that the *Laplacian* operator

$$\nabla^2 \equiv \partial_i \, \partial_i = \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_n^2} \tag{7.87}$$

is manifestly a scalar operator, and so if ϕ is a scalar, then so is $\nabla^2\phi$.

There is a special significance in tensor calculus to *antisymmetrised* derivatives of tensors. The most familiar example, in three dimensions, involves the antisymmetrised derivative of a vector, $\partial_i V_j - \partial_j V_i$. As in our discussion of the vector product, it is then convenient to take the Hodge dual of this, to obtain a vector. Thus one defines the curl operation, with the curl of a vector $\vec V$ being another vector (actually, of course, a pseudo-vector) $\vec X$, given by

$$\vec X \equiv \vec\nabla \times \vec V \, . \tag{7.88}$$

In components, this is just

$$X_i = \varepsilon_{ijk} \, \partial_j \, V_k \, . \tag{7.89}$$

In index notation one can easily prove various 3-dimensional identities, based on the fact that partial derivatives commute, $\partial_i \, \partial_j = \partial_j \, \partial_i$, such as

$$\vec\nabla \times \vec\nabla\phi = 0 \, , \qquad \vec\nabla \cdot (\vec\nabla \times \vec V) = 0 \, , \tag{7.90}$$

for any scalar ϕ and any vector $\vec V$. One can also immediately see from (7.60) that

$$\vec\nabla \times (\vec\nabla \times \vec V) = \vec\nabla \, (\vec\nabla \cdot \vec V) - \nabla^2 \, \vec V \, . \tag{7.91}$$