17 Motion on a Ring

To begin our study of the angular properties of the solutions of Schrödinger's equation, we consider the motion of a quantum particle of mass μ confined to move on a ring of constant radius r_0. As with classical orbits, let's assume that the ring lies in the x, y plane, so that in spherical coordinates $\theta = \frac{\pi}{2}$ =const. Then, since Ψ is independent of r and θ, derivatives with respect to those variables give zero and Schrödinger's equation reduces to

$$H_{\rm op}\Psi = -\frac{\hbar^2}{2\mu}\frac{1}{r_0^2}\frac{\partial^2}{\partial\phi^2}\Psi + U(r_0)\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{103}$$

Redoing the separation of variables procedure of the last section (see Practice Problem 1.3), and assuming that $\Psi = T(t)\Phi(\phi)$ only, we obtain the following separated ordinary differential equations

$$\frac{d^2\Phi}{d\phi^2} = -\frac{2I}{\hbar^2}\left(E - U(r_0)\right)\Phi \tag{104}$$

$$\frac{dT}{dt} = -\frac{i}{\hbar}ET \tag{105}$$

where we have used the substitution $\mu r_0^2 = I$, in which I would be the moment of inertia of a classical particle of mass μ traveling in a ring about the center-of-mass.

Alternatively, we could have obtained equations (104) and (105) from the results of our original separation of variables procedure (210), (99), (101), (102), by restricting the variables r and θ to the equator, noticing that the functions R and P are therefore constant, and that equation (99) reduces to:

$$A = \frac{2\mu}{\hbar^2}\left(E - U(r_0)\right) r_0^2$$

and equation (101) then reduces to:

$$B = -\frac{2\mu}{\hbar^2}\left(E - U(r_0)\right) r_0^2$$

Since the coefficient of Φ on the right-hand-side of (104) is a constant

$$\sqrt{\frac{2I}{\hbar^2}(E - U(r_0))} = \text{constant} \tag{106}$$

the solutions of the Φ equation (104), are

$$\Phi_m(\phi) \stackrel{\text{def}}{=} N\, e^{im\phi} \tag{107}$$

where

$$m = \pm\sqrt{\frac{2I}{\hbar^2}(E - U(r_0))} \tag{108}$$

and N is a normalization constant.

There is no "boundary" on the ring, on which we can impose boundary conditions. However, there is one very important property of the wave function that we can invoke: it must be single-valued. The variable ϕ is geometrically an angle, so that $\phi + 2\pi$ is physically the same point as ϕ. If we go once around the ring and return to our starting point, the value of the wave function must remain the same. Therefore the solutions must satisfy the periodicity condition $\Phi_m(\phi + 2\pi) = \Phi_m(\phi)$. This is impossible unless m is real so that the solutions are oscillatory, i.e. $E - U(r_0) > 0$. Furthermore, the solutions must have the correct period, i.e.

$$m \in \{0, \pm 1, \pm 2, \ldots\} \tag{109}$$

The quantum number m is called the *azimuthal* or *magnetic quantum number*. Note that the solution permits both positive and negative values of m as well as zero.

Solving (108) for the possible eigenvalues of energy, we obtain

$$E_m = \frac{\hbar^2}{2I}\, m^2 + U(r_0) \tag{110}$$

For this simplified ring problem, we can choose the potential energy $U(r_0)$ to be zero, but we will have to remember that we should not make this choice when we are working on the full hydrogen atom problem. There is a degeneracy that arises in this calculation. Note that the wave functions corresponding to $+|m|$ and $-|m|$ have the same energy but represent (as we will see) different states of the motion.

As usual, we choose the normalization N in (107) so that, if the particle is in an eigenstate, the probability of finding it somewhere on the ring is unity.

$$1 = \int_0^{2\pi} \Phi_m^*(\phi)\, \Phi_m(\phi)\, r_0 d\phi = \int_0^{2\pi} N^* e^{-im\phi}\, N e^{im\phi}\, r_0 d\phi = 2\pi r_0 |N|^2 \tag{111}$$

$$\Rightarrow \quad N = \frac{1}{\sqrt{2\pi r_0}} \tag{112}$$

This is a one-dimensional problem, just like the problem of a particle-in-a-box which you solved in the Waves Paradigm (now in ϕ instead of x) and the solutions have the same oscillatory form. Everything that you learned in that Paradigm is immediately applicable here. As in that problem, the energy eigenvalues are discrete because of a boundary condition. The only difference is that the boundary condition appropriate to this problem is periodicity, since ϕ is a physical angle, rather than $\Psi(x) = 0$ at the boundaries, appropriate to an infinite potential.

. . . .

1 Practice Problems

1. Show that (107) and (108) are solutions of (104).

2. Why is there a factor of r_0 in the integral in (111)?

. . . .

18 ANGULAR MOMENTUM OF THE PARTICLE ON A RING

Classically, a particle moving in a circle has an angular momentum perpendicular to the plane of the circle, which for a ring in the x, y–plane would be in the z direction. Since angular momentum is defined by $\vec{L} = \vec{r} \times \vec{p}$, we have $L_z = xp_y - yp_x$. To make the transition to quantum mechanics, we replace p_x and p_y by their operator equivalents:

$$L_z = xp_y - yp_x \Rightarrow x\frac{\hbar}{i}\frac{\partial}{\partial y} - y\frac{\hbar}{i}\frac{\partial}{\partial x} \tag{113}$$

Using a straightforward application of the chain rule (see Practice Problems, below) to replace the Cartesian partial derivatives with their polar representations, we obtain

$$\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial \phi} \tag{114}$$

The effect of operating on the ring eigenfunctions with this operator is:

$$\frac{\hbar}{i}\frac{\partial}{\partial\phi}\left(\frac{1}{\sqrt{2\pi}}\,e^{im\phi}\right) = m\hbar\left(\frac{1}{\sqrt{2\pi}}\,e^{im\phi}\right) \tag{115}$$

The energy eigenfunctions $\Phi_m(\phi)$ are thus also eigenfunctions of $\hat{L}_z$ with eigenvalues $m\hbar$. Because the $\Phi_m(\phi)$ are eigenfunctions of both energy and angular momentum, we can make simultaneous determinations of the eigenvalues of energy and angular momentum.

Considering the angular momentum helps us understand the degeneracy of the eigenfunctions with respect to energy. The $\pm m$ degeneracy of the energy eigenstates corresponds to $L_z = +m\hbar$ and $L_z = -m\hbar$. That is, the two degenerate states represent particles rotating in opposite directions around the ring.

For a classical particle rotating in a circular path in the x, y-plane, the kinetic energy is $T = \frac{1}{2}I\omega^2 = L_z^2/2I$, where I is the rotational inertia (moment of inertia). The rotational inertia of a single particle of mass μ moving in a circle of radius r_0 is $I = \mu r_0^2$. The Hamiltonian for the system is thus

$$H = T + U = \frac{L_z^2}{2I} + U = -\frac{\hbar^2}{2\mu r_0^2}\frac{\partial^2}{\partial\phi^2} + U_0 \tag{116}$$

It is apparent from this approach that the energy and the angular momentum have simultaneous eigenvalues because they are commuting operators. Clearly $[L_z^2, L_z] = 0$, so that E and L_z have the same eigenfunctions. Therefore, we see that (104) and (115) are the position-space representations of the eigenvalue equations

$$\hat{H}\,|m\rangle = E_m|m\rangle \tag{117}$$

$$\hat{L}_z\,|m\rangle = \hbar m\,|m\rangle \tag{118}$$

Because the Φ_m are simultaneous eigenstates of both $\hat{H}$ and $\hat{L}_z$, it is possible to make simultaneous measurements of both the energy and the z-component of angular momentum.

In setting up the problem of the particle on the ring, we constrained the motion to the x, y-plane, so that the angular momentum vector is in the z direction. However, according to quantum mechanics (yet another form of the Heisenberg uncertainty relationships) it is not possible to know the direction of the angular momentum vector. Our knowledge of the angular momentum vector is limited to its length and any one component. If the vector lies along the z-axis, then we would know all three of its components (the x and y components being zero). We'll see how the three-dimensional problem solves this contradiction.

. . . .

1 Practice Problems

1. Using a the chain rule for partial derivatives, show that (113) is indeed the same as (114), thereby showing that this operator is the quantum analogue of the z-component of angular momentum.

. . . .

19 TIME DEPENDENCE OF RING STATES

We know, from the theory of Fourier series, that we can write any initial probability distribution, which is necessarily periodic, as a sum of the energy eigenstates.

$$\Phi(\phi) = \sum_{m=-\infty}^{\infty} c_m \, \Phi_m(\phi) = \sum_{m=-\infty}^{\infty} c_m \left(\frac{1}{\sqrt{2\pi \, r_0}} \, e^{im\phi} \right) \tag{119}$$

where, for the probability distribution to be normalized, we must have:

$$\sum_{m=-\infty}^{\infty} |c_m|^2 = 1 \tag{120}$$

To find the time evolution of the eigenstates $\Phi_m(\phi)$, we must solve the t equation (105). Since, for each Φ_m, we have now found the value of the constant $E = E_m$, given by (110), we can solve (105) trivially.

$$T(t) = e^{-\frac{i}{\hbar} E_m t} \tag{121}$$

A deep theorem in the theory of partial differential equations states that if you have found an expansion of the initial probability density in terms of the eigenstates of the Hamiltonian, then the time evolution of that probability density is simply obtained by multiplying each eigenstate individually by the appropriate time evolution.

$$\Phi(\phi, t) = \sum_{m=-\infty}^{\infty} c_m \, \Phi_m(\phi) \, e^{-\frac{i}{\hbar} E_m t} \tag{122}$$

BE CAREFUL! There are an infinite number of different values for the energy, depending on the eigenstate of the Hamiltonian. It is incorrect to multiply the initial state (119) by a single over-all exponential time factor. Each term in the series gets its own time evolution.

20 Motion on a Sphere

We will now relax the restriction that the mass be confined to the ring, and instead, let it range over the surface of a sphere of radius r_0. The results of this analysis yield predictions that can be successfully compared with experiment for molecules and nuclei that rotate more than they vibrate. For this reason, the problem of a mass confined to a sphere is often called the rigid rotor problem. Furthermore, the solutions that we will find for equations (101) and (102), called spherical harmonics, will occur whenever one solves a partial differential equation that involves spherical symmetry.

For homework, you will write down the Schrödinger equation for a particle restricted to a sphere and use the separation of variables procedure to obtain an equivalent set of ordinary differential equations. One of the equations you obtain will be (102), with solutions exactly as we found them for the ring. The other equation will be (101) with slightly different labels for the unknown constants. So, to solve either Schrödinger's equation for the hydrogen atom or for a particle restricted to a sphere, we need to solve (101). This will be the job of the next five sections.

21 Change of Variables

Since we have solved the ϕ equation (102) and found the possible values of the separation constant $\sqrt{B} = m \in \{0, \pm 1, \pm 2, \ldots\}$, the θ equation becomes an eigenvalue/eigenfunction equation for the unknown separation constant A and the unknown function $P(\theta)$.

$$\left(\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - A\sin^2\theta - m^2\right) P(\theta) = 0 \tag{123}$$

We start with a change of independent variable $z = \cos\theta$ where z is the usual rectangular coordinate in three-space. As θ ranges from 0 to π, z ranges from 1 to -1. We see from Figure 4 that:

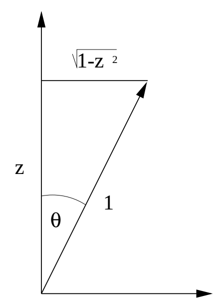

Figure 4: Relationship between z and θ.

$$\sqrt{1-z^2} = \sin\theta \tag{124}$$

Using the chain rule for partial derivatives, we have:

$$\frac{\partial}{\partial\theta} = \frac{\partial z}{\partial\theta}\frac{\partial}{\partial z} = -\sin\theta\frac{\partial}{\partial z} = -\sqrt{1-z^2}\frac{\partial}{\partial z} \tag{125}$$

Notice, particularly, the last equality: we are trying to change variables from θ to z, so it is important to make sure we change **all** the θ's to z's. Multiplying by $\sin\theta$ we obtain:

$$\sin\theta\frac{\partial}{\partial\theta} = -\left(1-z^2\right)\frac{\partial}{\partial z} \tag{126}$$

Be careful finding the second derivative; it involves a product rule:

$$\begin{aligned}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) &= \left(1-z^2\right)\frac{\partial}{\partial z}\left(\left(1-z^2\right)\frac{\partial}{\partial z}\right) \\ &= \left(1-z^2\right)^2\frac{\partial^2}{\partial z^2} - 2z\left(1-z^2\right)\frac{\partial}{\partial z}\end{aligned} \tag{127}$$

Inserting (124) and (127) into (123), we obtain a standard form of the Associated Legendre's equation:

$$\left(\left(1-z^2\right)\frac{\partial^2}{\partial z^2} - 2z\frac{\partial}{\partial z} - A - \frac{m^2}{(1-z^2)}\right) P(z) = 0 \tag{128}$$

In §22 and §25, we will solve this equation. After we have found the eigenfunctions $P(z)$, we will substitute $z = \cos\theta$ everywhere to find the eigenfunctions of the original equation (123).

22 SERIES SOLUTIONS OF ODE'S

The simplest possible ϕ–dependence on the ring is, of course, $\Phi(\phi) = \text{constant}$, which corresponds in equation (123) to $m = 0$. We will first find solutions for this special case, which is known as *Legendre's equation.*

$$\left(\left(1-z^2\right)\frac{\partial^2}{\partial z^2} - 2z\frac{\partial}{\partial z} - A\right) P(z) = 0 \tag{129}$$

Let's use series methods to find a solution of (129), i.e. let's assume that the solution can be written as a Taylor series

$$P(z) = \sum_{n=0}^{\infty} a_n\, z^n \tag{130}$$

and solve for the coefficients a_n. Then we have

$$\frac{dP}{dz} = \sum_{n=0}^{\infty} a_n\, n\, z^{n-1} \tag{131}$$

$$\frac{d^2P}{dz^2} = \sum_{n=0}^{\infty} a_n\, n(n-1)\, z^{n-2} \tag{132}$$

and then plug (130)–(132) into (129) to obtain

$$0 = \sum_{n=0}^{\infty} a_n\, n(n-1)\, z^{n-2} - z^2 \sum_{n=0}^{\infty} a_n\, n(n-1)\, z^{n-2} - 2z \sum_{n=0}^{\infty} a_n\, n\, z^{n-1} - A \sum_{n=0}^{\infty} a_n\, z^n \tag{133}$$

In (133), the summation variable n is a dummy variable (just like a dummy variable of integration). Therefore, in the first sum, we can shift $n \to n+2$.

$$\sum_{n=0}^{\infty} a_n\, n(n-1)\, z^{n-2}$$

$$
\begin{aligned}
\rightarrow\quad & \sum_{n=-2}^{\infty} a_{n+2}(n+2)(n+1)z^n \\
= \quad & a_{-2}(-2+2)(-2+1)z^{-2} + a_{-1}(-1+2)(-1+1)z^{-1} + \sum_{n=0}^{\infty} a_{n+2}(n+2)(n+1)z^n \\
= \quad & \sum_{n=0}^{\infty} a_{n+2}(n+2)(n+1)z^n
\end{aligned}
$$

Pay special attention to what happened to the lower limit of the sum. The new sum would start at $n = -2$, but since the factor of $(n+2)$ in the first term and the factor of $(n+1)$ in the second term means that these terms are zero and we can eliminate them from the sum. At the same time, bring any overall factors of z into the corresponding sums. Finally, since each sum now has a factor of z^n and runs over the same range, group the sums together.

$$
\sum_{n=-2}^{\infty} a_{n+2}\,(n+2)(n+1)\,z^n - \sum_{n=0}^{\infty} a_n\,n(n-1)\,z^n - 2\sum_{n=0}^{\infty} a_n\,n\,z^n - A\sum_{n=0}^{\infty} a_n\,z^n \tag{134}
$$

$$
= \sum_{n=0}^{\infty} \left[a_{n+2}\,(n+2)(n+1) - a_n\,n(n-1) - 2\,a_n\,n - A\,a_n\right] z^n = 0 \tag{135}
$$

Now comes the MAGIC part. Since (135) is true *for all values of z*, the coefficient of z^n for each term in the sum must separately be zero, i.e.

$$
a_{n+2}\,(n+2)(n+1) - a_n\,n(n-1) - 2\,a_n\,n - A\,a_n = 0 \tag{136}
$$

and therefore we can solve for a_{n+2} in terms of a_n

$$
a_{n+2} = \frac{n(n+1)+A}{(n+2)(n+1)}\,a_n \tag{137}
$$

By plugging successive even values of n into the recurrence relation (137) allows us to find a_2, a_4, etc. in terms of the arbitrary constant a_0 and successive odd values of n allow us to find a_3, a_5, etc. in terms of the arbitrary constant a_1. Thus, for the second order differential equation (129) we obtain two solutions as expected. a_0 becomes the normalization constant for a solution with only even powers of z and a_1 becomes the normalization constant for a solution with only odd powers of z. For example:

$$
a_2 = \frac{A}{2}\,a_0 \tag{138}
$$

$$
\begin{aligned}
a_4 &= \frac{6+A}{12}\, a_2 = \left(\frac{6+A}{12}\right)\left(\frac{A}{2}\right) a_0 \qquad \text{etc.} && (139)\\
a_3 &= \frac{2+A}{6}\, a_1 && (140)\\
a_5 &= \frac{12+A}{20}\, a_2 = \left(\frac{12+A}{20}\right)\left(\frac{6+A}{12}\right) a_0 \qquad \text{etc.} && (141)
\end{aligned}
$$

so that

$$
\begin{aligned}
P(z) &= a_0 \left[\frac{A}{2}\, z^0 + \left(\frac{6+A}{12}\right)\left(\frac{A}{2}\right) z^2 + \ldots\right] && (142)\\
&+ a_1 \left[\frac{2+A}{6}\, z^1 + \left(\frac{12+A}{20}\right)\left(\frac{2+A}{6}\right) z^3 + \ldots\right] && (143)
\end{aligned}
$$

In general, the solutions of an ordinary linear differential equation can blow-up only where the coefficients of the equation itself are singular, in this case at $z = \pm 1$, which correspond to the north and south poles $\theta = 0, \pi$. But there is nothing special about physics at these points, only the choice of coordinates is special there. Therefore, we want to choose solutions of (129) which are regular (non-infinite) at $z = \pm 1$. This is an important example of a problem where the choice of coordinates for a partial differential equation end up imposing boundary conditions on the ordinary differential equation which comes from it. Therefore, the infinite series (130) could possibly blow up at the endpoints $z = \pm 1$, but a polynomial could not. So if we choose the special values for the separation constant A to be $A = -\ell(\ell+1)$ where ℓ is a non-negative integer, we see from (137) that for $n \geq \ell$ the coefficients become zero and the series terminates in a polynomial. The solutions for these special values of A are polynomials of degree ℓ, denoted P_ℓ, and called Legendre polynomials.

23 LEGENDRE POLYNOMIALS

It turns out that the Legendre polynomials can also be found from Rodrigues' formula

$$
P_\ell(z) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dz^\ell} \left(z^2 - 1\right)^\ell \tag{144}
$$

(The proof is lengthy, but beautiful. Ask!) Rodrigues' Formula can be used to generate solutions quickly. To do this, write

$$
\left(z^2 - 1\right)^\ell = (z-1)^\ell (z+1)^\ell = a^\ell b^\ell \tag{145}
$$

and use the product rule

$$
\begin{aligned}
\frac{d^\ell}{dz^\ell}\left(z^2-1\right)^\ell &= \left(\frac{d^\ell a^\ell}{dz^\ell}\right) b^\ell + \ell\left(\frac{d^{\ell-1}a^\ell}{dz^{\ell-1}}\right)\left(\frac{db^\ell}{dz}\right) \\
&\quad + \frac{\ell(\ell-1)}{2!}\left(\frac{d^{\ell-2}a^\ell}{dz^{\ell-2}}\right)\left(\frac{d^2 b^\ell}{dz^2}\right) + \ldots + a^\ell\left(\frac{d^\ell b^\ell}{dz^\ell}\right)
\end{aligned} \tag{146}
$$

where the coefficient of the i^{th} term in the product rule is the binomial coefficient

$$
\binom{\ell}{i} = \binom{\ell}{\ell-i} = \frac{\ell!}{(\ell-i)!\,i!} \tag{147}
$$

The first few Legendre polynomials are:

$$
\begin{aligned}
P_0(z) &= 1 & (148)\\
P_1(z) &= z & (149)\\
P_2(z) &= \frac{1}{2}(3z^2-1) & (150)\\
P_3(z) &= \frac{1}{2}(5z^3-3z) & (151)\\
P_4(z) &= \frac{1}{8}(35z^4-30z^2+3) & (152)\\
P_5(z) &= \frac{1}{8}(63z^5-70z^3+15z) & (153)
\end{aligned}
$$

There are several useful patterns to the Legendre polynomials:

- The overall coefficient for each solution is conventionally chosen so that $P_\ell(1) = 1$. *As discussed in the next section, this is an inconvenient convention that we are stuck with!*
- $P_\ell(z)$ is a polynomial of degree ℓ.
- Each $P_\ell(z)$ contains only odd or only even powers of z, depending on whether ℓ is even or odd. Therefore, each $P_\ell(z)$ is either an even or an odd function.
- Since the differential operator in (129) is Hermitian (unproven), we are guaranteed by a deep theorem of mathematics that the Legendre

polynomials are orthogonal for different values of ℓ (just as with Fourier series) [1] , i.e.

$$\int_{-1}^{1} P_k^*(z)\, P_\ell(z)\, dz = \frac{\delta_{k\ell}}{\ell + \frac{1}{2}} \tag{154}$$

The "squared norm" of P_ℓ is just $1/(\ell + \frac{1}{2})$. To normalize each $P_\ell(z)$ it should be multiplied by $\sqrt{\ell + \frac{1}{2}}$.

Notice that the differential equation

$$\frac{\partial^2 P}{\partial z^2} - \frac{2z}{1-z^2}\frac{\partial P}{\partial z} + \frac{\ell(\ell+1)}{1-z^2}P = 0 \tag{155}$$

is a **different** equation for different values of ℓ. For a given value of ℓ, you should expect two solutions of (155). Why? We have only given one. It turns out that the "other" solution for each value of ℓ is not regular (i.e. it blows up) at $z = \pm 1$. In cases where the separation constant A does not have the special value $l(l+1)$ for non-negative integer values of ℓ, it turns out that *both* solutions blow up. We discard these irregular solutions as unphysical for the problem we are solving.

. . . .

1 Practice Problems

1. Use Rodrigues' formula, by hand, to find the first 5 Legendre polynomials.

2. Go through the worksheet `legendre.mws`. You do not need to turn anything in. However, there are two things you should get out of this worksheet:

   (a) Get a feel for what the Legendre polynomials look like. There are some questions in the worksheet to help guide your exploration.

   (b) Learn the syntax for writing a "loop" in Maple. There is a discussion of this in the worksheet. Loops are one of the most useful of all computer programming techniques.

. . . .

[1] One shows this using Rodrigues' Formula and repeated integration by parts, noting that the "surface terms" always vanish.

24 LEGENDRE POLYNOMIAL SERIES

There is a very powerful mathematical theorem which says that *any* sufficiently smooth function $f(z)$, defined on the interval $-1 < z < 1$, can be expanded as a linear combination of Legendre polynomials

$$f(z) = \sum_{\ell=0}^{\infty} c_\ell \, P_\ell(z) \tag{156}$$

(This theorem is the analogue of the theorem which says that any sufficiently smooth periodic function can be expanded in a Fourier series.) You will have several occasions in physics to expand functions in Legendre polynomial series, so we will explore the technique in this section.

We can find the coefficients c_ℓ by taking the inner product of both sides of (156) in turn with each "basis vector" P_k and using (154). This yields

$$\int_{-1}^{1} P_k^*(z)\, f(z)\, dz = \int_{-1}^{1} P_k^*(z) \sum_{\ell=0}^{\infty} c_\ell \, P_\ell(z)\, dz \tag{157}$$

$$= \sum_{\ell=0}^{\infty} c_\ell \int_{-1}^{1} P_k^*(z)\, P_\ell(z)\, dz \tag{158}$$

$$= \sum_{\ell=0}^{\infty} c_\ell \, \frac{\delta_{k\ell}}{\ell + \frac{1}{2}} \tag{159}$$

$$= \frac{c_k}{k + \frac{1}{2}} \tag{160}$$

or equivalently

$$c_k = \left(k + \frac{1}{2}\right) \int_{-1}^{1} P_k^*(z)\, f(z)\, dz \tag{161}$$

This expression should be compared with the exponential version of a Fourier series for $f(z)$ on the same interval $-1 \le z \le 1$, namely

$$f(z) = \sum_{n=-\infty}^{\infty} C_n \, e^{in\pi z} \tag{162}$$

where

$$C_n = \frac{1}{2}\int_{-1}^{1} e^{-in\pi z} f(z)\,dz \tag{163}$$

Note the analogous role played by the *normalization constants* $k+\frac{1}{2}$ and $\frac{1}{2}$. If we had made an unconventional, but more convenient, choice for the normalization for the Legendre polynomials such that the value of the integrals in (154) were simply $\delta_{k\ell}$, then we would not need to carry around the extra factor of $k+\frac{1}{2}$ in (161).

1 Example: Legendre Expansion of $\varepsilon(z)$

Consider the step function

$$\varepsilon(z) = 2\,\Theta(z) - 1 = \begin{cases} +1 & (z>0) \\ -1 & (z<0) \end{cases} \tag{164}$$

where Θ is the Heaviside step function; note that $\varepsilon(z)$ is an *odd* function of z. Using (161) leads to

$$\begin{aligned} c_\ell &= \left(\ell+\frac{1}{2}\right)\int_{-1}^{1} P_\ell^*(z)\,\varepsilon(z)\,dz && (165) \\ &= -\left(\ell+\frac{1}{2}\right)\int_{-1}^{0} P_\ell^*(z)\,dz + \left(\ell+\frac{1}{2}\right)\int_{0}^{1} P_\ell^*(z)\,dz && (166) \end{aligned}$$

and each integral in the final expression is an elementary integral of a polynomial. Furthermore, it is easily seen that these two integrals cancel if ℓ is even, and add if ℓ is odd, so that

$$c_\ell = \begin{cases} 0 & (\ell \text{ even}) \\ 2\left(\ell+\frac{1}{2}\right)\displaystyle\int_{0}^{1} P_\ell^*(z)\,dz & (\ell \text{ odd}) \end{cases} \tag{167}$$

These coefficients are easily evaluated on Maple for as many values of ℓ as desired.

25 ASSOCIATED LEGENDRE FUNCTIONS

We now return to equation (128) to consider the cases with $m \neq 0$. We can solve these equations with (a slightly more sophisticated version of) the series techniques from the $m = 0$ case. We would again find solutions that are regular at $z = \pm 1$ whenever we choose $A = -\ell(\ell+1)$ for $\ell \in \{0, 1, 2, 3, \ldots\}$. With this value for A, we obtain the standard form of Legendre's associated equation, namely

$$\left(\frac{\partial^2}{\partial z^2} - \frac{2z}{1-z^2}\frac{\partial}{\partial z} + \frac{\ell(\ell+1)}{1-z^2} - \frac{m^2}{(1-z^2)^2} \right) P(z) = 0 \qquad (168)$$

Recall that this equation was obtained by separating variables in spherical coordinates. Solutions of this equation which are regular at $z = \pm 1$ are called *associated Legendre functions*, and turn out to be given by

$$P_\ell^m(z) = P_\ell^{-m}(z) = (1-z^2)^{m/2}\frac{d^m}{dz^m}\left(P_\ell(z)\right) \qquad (169)$$

$$= (1-z^2)^{m/2}\frac{d^{m+\ell}}{dz^{m+\ell}}\left((z^2-1)^\ell\right) \qquad (170)$$

where $m \geq 0$. [2] Note that if $z = \cos\theta$, then $P_\ell(z)$ is a polynomial in $\cos\theta$, while

$$(1-z^2)^{m/2} = (\sin^2\theta)^{m/2} = \sin^m\theta \qquad (171)$$

so that $P_\ell^m(z)$ is a polynomial in $\cos\theta$ times a factor of $\sin^m\theta$. Some other properties of the associated Legendre functions are

- $P_\ell^m(z) = 0$ if $|m| > \ell$
- $P_\ell^{-m}(z) = P_\ell^m(z)$
- $P_\ell^m(\pm 1) = 0$ for $m \neq 0$ (cf. factor of $(1-z^2)^{m/2}$)
- $P_\ell^m(-z) = (-1)^{\ell-m}P_\ell^m(z)$ (behavior under parity)
- $\displaystyle\int_{-1}^{1} P_\ell^m(z)P_q^m(z)\,dz = \frac{2}{(2\ell+1)}\frac{(\ell+m)!}{(\ell-m)!}\,\delta_{\ell q}$

The last property shows that for each given value of m, the Associated Legendre functions form an orthonormal basis on the interval $-1 \leq z \leq 1$. Any function on this interval can be expanded in terms of anyone of these bases.

[2] Some authors define $P_\ell^{-m}(z)$ with a different phase.

26 SPHERICAL HARMONICS

We have found that normalized solutions of the ϕ equation (102) satisfying periodic boundary conditions are

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}}\, e^{im\phi} \qquad\qquad (m = 0, \pm 1, \pm 2, ...) \tag{172}$$

and normalized solutions of the θ equation (101 which are regular at the poles are given by

$$P(\cos\theta) = \sqrt{\frac{(2\ell+1)}{2}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\, P_\ell^m(\cos\theta) \tag{173}$$

Combining these yields via multiplication (we assumed solutions of this type when we first did the separation of variables procedure), we obtain the *spherical harmonics*

$$Y_\ell^m(\theta,\phi) = (-1)^{(m+|m|)/2}\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\, P_\ell^m(\cos\theta)\, e^{im\phi} \tag{174}$$

where the somewhat peculiar choice of phase is conventional.

The spherical harmonics are orthonormal on the unit sphere:

$$\int_0^{2\pi}\int_0^{\pi} \left(Y_{\ell_1}^{m_1}\right)^* Y_{\ell_2}^{m_2} \sin\theta\, d\theta\, d\phi = \delta_{\ell_1\ell_2}\delta_{m_1 m_2} \tag{175}$$

since $dz = \sin\theta\, d\theta$. They are complete in the sense that any sufficiently smooth function f on the unit sphere can be expanded in a *Laplace series* as

$$f(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} a_{\ell m}\, Y_\ell^m(\theta,\phi) \tag{176}$$

where

$$a_{\ell m} = \int_0^{2\pi}\int_0^{\pi} (Y_\ell^m)^*\, f(\theta,\phi)\, \sin\theta\, d\theta\, d\phi \tag{177}$$

1 Example

Suppose you want a function of (θ, ϕ) which satisfies

$$f(\theta, \phi) = \begin{cases} \sin\theta & 0 < \theta < \frac{\pi}{2} \\ 0 & \text{otherwise} \end{cases} \tag{178}$$

Then f takes the form (176), and the constants $a_{\ell m}$ can be determined from (177), yielding

$$a_{\ell m} = \int_0^{2\pi} \int_0^{\pi/2} (Y_\ell^m)^* \sin^2\theta \, d\theta \, d\phi \tag{179}$$

$$= N_{\ell m} \int_0^{2\pi} e^{-im\phi} \, d\phi \int_0^{\pi/2} P_\ell^m(\cos\theta) \sin^2\theta \, d\theta \tag{180}$$

where

$$N_{\ell m} = (-1)^{(m+|m|)/2} \sqrt{\frac{(2\ell+1)}{4\pi} \frac{(\ell-|m|)!}{(\ell+|m|)!}} \tag{181}$$

Thus,

$$a_{\ell m} = \begin{cases} 0 & (m \neq 0) \\ \sqrt{(2\ell+1)\pi} \displaystyle\int_0^{\pi/2} P_\ell(\cos\theta) \sin^2\theta \, d\theta & (m = 0) \end{cases} \tag{182}$$

For $m = 0$, the integral is most easily computed with the substitution $z = \cos\theta$; the first few coefficients are:

$$\begin{aligned} a_{00} &= \frac{\pi}{8} \qquad a_{10} = \frac{1}{2} \qquad a_{20} = -\frac{5\pi}{64} \\ a_{30} &= -\frac{7}{12} \qquad a_{40} = -\frac{9\pi}{512} \qquad a_{50} = \frac{77}{240} \end{aligned} \tag{183}$$

(each of which should be multiplied by $\sqrt{4\pi/(2\ell+1)}$). As you can check by graphing, however, it requires at least twice this many terms to obtain a good approximation.