Series Solution

Lecture 22

Physics 342
Quantum Mechanics I

Wednesday, March 24th, 2008

22.1 Introduction

The series method for solving ODEs (Frobenius's method) is a powerful tool, and one which we shall use over and over in our quantum mechanical studies. It shows up naturally in the context of spherical separation of variables, where you saw it last semester in E&M. We will review the Legendre series expansion approach for the azimuthally symmetric (no ϕ dependence) solution to Laplace's equation, then connect the "associated Legendre series", which solves the problem for non-trivial ϕ dependence, to the Legendre series.

Finally, as another example of the series approach, we will look back at the harmonic oscillator problem. The eigenvalue problem there is similar to the ones we encounter for the radial part of Schrödinger's equation in spherical coordinates.

22.2 The Angular Equation(s)

The (multiplicatively) separated Laplacian in spherical coordinates is

$$\nabla^2(f(r)\,g(\theta)\,h(\phi)) = \frac{1}{r^2}\frac{d}{dr}\left(r^2 f'\right)\,g\,h + \frac{1}{r^2\,\sin\theta}\frac{d}{d\theta}\left(\sin\theta\,g'\right)\,f\,h + \frac{1}{r^2\,\sin^2\theta}\,h''\,f\,g, \tag{22.1}$$

where primes denote derivatives w.r.t. the necessarily single argument of each of the relevant functions. When we solve Laplace's equation, $\nabla^2(f\,g\,h) = 0$, we can isolate these terms in terms of their dependence:

$$0 = \frac{1}{f}\left[\frac{d}{dr}\left(r^2\,f'\right)\right] + \left[\frac{1}{g}\,\frac{1}{\sin\theta}\,\frac{d}{d\theta}\left(\sin\theta\,g'\right) + \frac{1}{\sin^2\theta}\,\frac{h''}{h}\right] \tag{22.2}$$

and we typically separate by setting:

$$\begin{aligned} \ell\,(\ell+1) &= \frac{1}{f}\,\left[\frac{d}{dr}\,(r^2\,f')\right] \\ -\ell\,(\ell+1) &= \left[\frac{1}{g}\,\frac{1}{\sin\theta}\,\frac{d}{d\theta}\,\left(\sin\theta\,g'\right) + \frac{1}{\sin^2\theta}\,\frac{h''}{h}\right]. \end{aligned} \tag{22.3}$$

Now taking the angular portion, we can split further:

$$-\ell\,(\ell+1)\sin^2\theta = \left[\frac{1}{g}\,\sin\theta\,\frac{d}{d\theta}\,\left(\sin\theta\,g'\right)\right] + \left[\frac{h''}{h}\right]. \tag{22.4}$$

Of the three terms in the above expression, two depend on θ, and $\frac{h''}{h}$ is a function only of ϕ. Set:

$$\begin{aligned} -m^2 &= \frac{h''}{h} \longrightarrow h(\phi) = A\,e^{i\,m\,\phi} \\ m^2 &= \frac{1}{g}\,\sin\theta\,\frac{d}{d\theta}\,\left(\sin\theta\,g'\right) + \ell\,(\ell+1)\,\sin^2\theta. \end{aligned} \tag{22.5}$$

22.3 The Case $m = 0$

If we take the azimuthally symmetric case, with $m = 0$, so that $f(r)\,g(\theta)\,h(\phi) = f(r)\,g(\theta)$, our ODE simplifies:

$$\sin\theta\,\frac{d}{d\theta}\,\left(\sin\theta\,g'\right) + \ell\,(\ell+1)\,\sin^2\theta\,g = 0. \tag{22.6}$$

In order to get rid of the explicit trigonometric functions, suppose we take $g(\theta) = g(z)$ with $z = \cos\theta$. We can make the change, induced by the chain rule:

$$\frac{d}{d\theta}\,g(z) = -\sin\theta\,\frac{dg}{dz} \qquad \frac{d}{d\theta} \longrightarrow -\sin\theta\,\frac{d}{dz}. \tag{22.7}$$

Making this substitution, and noting that $\sin^2\theta = 1 - z^2$, we have the equivalent ODE:

$$\frac{d}{dz}\left((1-z^2)\,\frac{dg(z)}{dz}\right) + \ell\,(\ell+1)\;g(z) = 0. \tag{22.8}$$

We know that $z \in [-1, 1]$, so it is a restricted argument. But that aside, the above is, literally begging for a series approach.

Writing out all terms explicitly, and setting $g' \equiv g'(z) = \frac{dg(z)}{dz}$ for visual clarity, our target equation is

$$(1 - z^2)\, g'' - 2\, z\, g' + \ell\,(\ell + 1)\ g = 0. \tag{22.9}$$

The Frobenius ansatz for $g(z)$ is:

$$g(z) = z^p \sum_{j=0}^{\infty} \alpha_j\, z^j, \tag{22.10}$$

then the derivative and second derivative are

$$\begin{aligned} g'(z) &= z^p \sum_{j=0}^{\infty} \alpha_j\,(j+p)\ z^{j-1} \\ g''(z) &= z^p \sum_{j=0}^{\infty} \alpha_j\,(j+p)\,(j+p-1)\ z^{j-2}. \end{aligned} \tag{22.11}$$

If we input these expansions in (22.9), we get:

$$\begin{aligned} 0 = z^p \Bigg\{ &\sum_{j=0}^{\infty} \alpha_j\,(j+p)\,(j+p-1)\ z^{j-2} + \sum_{j=0}^{\infty} (-\alpha_j)\,(j+p)\,(j+p-1)\ z^j \\ &+ \sum_{j=0}^{\infty} (-2\,\alpha_j)\,(j+p)\ z^j + \sum_{j=0}^{\infty} (\ell\,(\ell+1)\ \alpha_j)\ z^j \Bigg\}. \end{aligned} \tag{22.12}$$

The first term is the only problematic one – set $k = j - 2$, then

$$\sum_{j=0}^{\infty} \alpha_j\,(j+p)\,(j+p-1)\ z^{j-2} = \sum_{k=-2}^{\infty} \alpha_{q+2}\,(k+p+2)\,(k+p+1)\ z^k \tag{22.13}$$

and we see that there are two unbalanced terms in this sum, namely the $k = -2$ and -1 contributions. If we pull out these two terms and re-label $k \to j$ (k is a dummy index), we have the following requirements:

$$\begin{aligned} 0 = \alpha_0\, p\,(p-1) z^{-2} + \alpha_1\,(p+1)\, p\, z^{-1} + \Bigg\{ \sum_{j=0}^{\infty} \Bigg[&\alpha_{j+2}\,(j+p+2)\,(j+p+1) \\ &- [(j+p)\,(j+p-1) + 2\,(j+p) - \ell\,(\ell+1)]\ \alpha_j \Bigg]\, z^j \Bigg\}. \end{aligned} \tag{22.14}$$

The first two terms must each be zero and this can be used to set p, and then the vanishing of each term in the sum provides a recursion relation. For example, if we take $p = 0$, and set $\alpha_1 = 0$, then our recursion is:

$$\begin{aligned}
\alpha_{j+2} &= \frac{(j+p)\,(j+p-1) + 2\,(j+p) - \ell\,(\ell+1)}{(j+p+2)\,(j+p+1)}\,\alpha_j \\
&= \frac{j\,(j+1) - \ell\,(\ell+1)}{(j+2)\,(j+1)}\,\alpha_j \\
&= \frac{(j+\ell+1)\,(j-\ell)}{(j+1)\,(j+2)}\,\alpha_j.
\end{aligned} \tag{22.15}$$

This recursion relation can start with $\alpha_0 = 0$ or $\alpha_1 = 0$. We then get even or odd solutions. We'll start with $\alpha_1 = 0$, and leave α_0 free to provide an eventual normalization. Consider the case $\ell = 1$, we have:

$$g(z) = -\sum_{j=0}^{\infty} \frac{1}{(2\,j+1)}\,z^{2j}. \tag{22.16}$$

This series becomes (the odd portion of) the harmonic series for $z = 1$, and that does not converge. So we have the "usual" sort of argument – since the infinite series does not converge for $z = \pm 1$, it must truncate (or we do not have an appropriate solution). Because we will have $z = \pm 1$ at the poles of the sphere, we have a family of polynomials – the α_{j+2} coefficient is zero when:

$$(j+\ell+1)\,(j-\ell) = 0 \longrightarrow j = \ell. \tag{22.17}$$

Note that this also imposes the restriction, $\ell \in \mathbb{Z}$.

The first few Legendre polynomials are listed below –

$$\begin{aligned}
P_0(z) &= \alpha_0 \\
P_2(z) &= \alpha_0\big(1 - 3\,z^2\big) \\
P_4(z) &= \alpha_0\left(1 - 10z^2 + \frac{35}{3}\,z^4\right) \\
&\;\;\vdots
\end{aligned} \tag{22.18}$$

There are a few observations we might make at this point – most notable: These series are all even functions of z, where are the odd solutions? A second observation might be – what a strange looking set of polynomials.

22.3.1 Odd Solutions

We have another option for $p = 0$, namely $\alpha_0 = 0$ with α_1 un-fixed. This gives us, once again, a class of solutions that do not converge at $z = \pm 1$, so we truncate at $j = \ell$ – this time, though, all the j values are odd, starting with $j = 1$, and incrementing by 2. The same recursion formula (22.15) holds in this case. If we leave the α_1 un-fixed, then the odd Legendre polynomials are:

$$\begin{aligned} P_1(z) &= \alpha_1 \, z \\ P_3(z) &= \alpha_1 \left(z - \frac{5}{3} \, z^3 \right) \\ P_5(z) &= \alpha_1 \left(z - \frac{14}{3} \, z^3 + \frac{21}{5} \, z^5 \right) \\ &\vdots \end{aligned} \tag{22.19}$$

Once again, we recover the harmonic series for ℓ even, $z = \pm 1$, and we conclude that we are to take the (necessarily truncated) even Legendre polynomials from above when ℓ is even, and this odd set when ℓ is odd. In order to get a convergent result, then, we must also require that $\ell \in \mathbb{Z}$.

22.4 Gauss's Test

We have motivated the notion that the Legendre series expansion does not converge for $z = \pm 1$, and particular values of ℓ, but we can use Gauss's test directly to prove it. Gauss's test reads, in our context – If

$$\frac{\beta_j}{\beta_{j+1}} = 1 + \frac{h}{j} + \frac{B(j)}{(j)^2} \tag{22.20}$$

for $B(j)$ a bounded function as $j \to \infty$, then $\sum_{j=0}^{\infty} \beta_j$ converges for $h > 1$, and diverges for $h \leq 1$.

Gauss's test applies when the coefficients are all positive, and we need to be a little careful here – if we write:

$$\alpha_{j+2} = \frac{j\,(j+1) - \ell\,(\ell+1)}{(j+1)\,(j+2)} \, \alpha_j \tag{22.21}$$

then there will be negative coefficients when $j < \ell$, but for $j > \ell$, we still have an infinite series, and all coefficients have the same sign, so we are working on that portion of the series that occurs for $j > \ell$.

Take $\beta_j = \alpha_{2j}$, then

$$\begin{aligned}\frac{\alpha_{2j}}{\alpha_{2(j+1)}} &= \frac{(2\,j+1)\,(2\,j+2)}{2\,j\,(2\,j+1)-\ell\,(\ell+1)} \\ &\approx 1+\frac{1}{j}+\frac{\frac{1}{4}\,\ell\,(\ell+1)}{j^2}+O\left(\frac{1}{j^3}\right).\end{aligned} \tag{22.22}$$

The expansion tells us that $B(j) \sim \frac{1}{j^2}$, so we know that $B(j)$ satisfies our assumption as $j \to \infty$. The coefficient $h = 1$, and then Gauss's test tells us that the series diverges. This series is precisely the sum given by setting $z = 1$, so we know that the Legendre series will diverge for $z = 1$, hence the necessity of truncation.

22.5 Orthogonality

The Legendre polynomials defined by the above recursion relation and denoted $P_\ell(z)$ are defined on $z \in [-1, 1]$, and satisfy (by explicit construction) the ODE:

$$(1-z^2)P_\ell''(z) - 2\,z\,P_\ell'(z) + \ell\,(\ell+1)\;P_\ell(z) = 0. \tag{22.23}$$

From this, we can show that the inner product of two Legendre polynomials:

$$P_\ell \cdot P_{\ell'} = \int_{-1}^{1} P_\ell^*(x)\,P_{\ell'}\,dx = 0 \tag{22.24}$$

unless $\ell = \ell'$.

Multiply the ODE for P_ℓ by $P_{\ell'}$ and vice versa:

$$\begin{aligned}0 &= (1-z^2)\,P_{\ell'}\,P_\ell'' - 2\,z\,P_{\ell'}\,P_\ell' + \ell\,(\ell+1)\;P_{\ell'}\,P_\ell \\ 0 &= (1-z^2)\,P_\ell\,P_{\ell'}'' - 2\,z\,P_\ell\,P_{\ell'}' + \ell'\,\left(\ell'+1\right)\;P_\ell\,P_{\ell'},\end{aligned} \tag{22.25}$$

and subtracting these two gives:

$$\begin{aligned}0 &= (1-z^2)\;\left[P_{\ell'}\,P_\ell'' - P_\ell\,P_{\ell'}''\right] - 2\,z\;\left[P_{\ell'}\,P_\ell' - P_\ell\,P_{\ell'}'\right] + \big(\ell\,(\ell+1) - \ell'\,\left(\ell'+1\right)\big)\;P_{\ell'}\,P_\ell \\ &= \frac{d}{dz}\;\left[(1-z^2)\left(P_{\ell'}\,P_\ell' - P_\ell\,P_{\ell'}'\right)\right] + \big(\ell\,(\ell+1) - \ell'\,\left(\ell'+1\right)\big)\;P_{\ell'}\,P_\ell.\end{aligned} \tag{22.26}$$

Finally, if we integrate this expression from $z = -1 \to 1$, the first term dies, since the Legendre polynomials are finite at $z = \pm 1$, and $(1-z^2)|_{-1}^{1} = 0$, we are left with:

$$\int_{-1}^{1} P_{\ell'}\,P_\ell\,dz = 0, \tag{22.27}$$

unless $\ell = \ell'$, in which case the integral need not vanish.

In order to find the dot product: $P_\ell \cdot P_\ell$ to set the normalization, we note that the generating function for the Legendre polynomials is:

$$G(z, \gamma) = \frac{1}{\sqrt{1 - 2\, z\, \gamma + \gamma^2}} = \sum_{j=0}^{\infty} \gamma^j\, P_j(z) \tag{22.28}$$

for $|\gamma| < 1$ (try Taylor expanding $G(z, \gamma)$ for γ small). The generating function can be used to develop "recursion relations" between the various Legendre polynomials. For example, if we take the γ and z partials of G,

$$\frac{\partial G}{\partial \gamma} = \frac{\gamma - z}{(1 - 2\, z\, \gamma + \gamma^2)}\, G(z, \gamma) \qquad \frac{\partial G}{\partial z} = \frac{-\gamma}{(1 - 2\, z\, \gamma + \gamma^2)}\, G(z, \gamma), \tag{22.29}$$

then we learn that

$$\frac{\partial G}{\partial z} = -\frac{\gamma}{\gamma - z}\, \frac{\partial G}{\partial \gamma}. \tag{22.30}$$

Using the infinite sum form, this relation is

$$\sum_{j=0}^{\infty} \gamma^{j+1}\, P_j' - \sum_{j=0}^{\infty} z\, \gamma^j\, P_j' + \sum_{j=0}^{\infty} \gamma^j\, j\, P_j = 0, \tag{22.31}$$

and re-labelling so as to collect powers of γ (which must individually vanish)

$$\sum_{j=1}^{\infty} \left(P_{j-1}' - z\, P_j' + j\, P_j\right)\, \gamma^j = 0 \tag{22.32}$$

we obtain the recursion relation:

$$\boxed{z\, P_j' - P_{j-1}' = j\, P_j.} \tag{22.33}$$

Now we can multiply this relation by P_j and integrate to find the normalization constant:

$$\int_{-1}^{1} z\, P_j'\, P_j\, dz - \int_{-1}^{1} P_{j-1}'\, P_j\, dz = j \int_{-1}^{1} (P_j)^2\, dz. \tag{22.34}$$

Taking each term in turn – we have

$$\int_{-1}^{1} z\, P_j\, P_j'\, dz = \frac{1}{2}\, P_j^2\, z\Big|_{z=-1}^{1} - \frac{1}{2} \int_{-1}^{1} P_j^2\, dz \tag{22.35}$$

and the Legendre polynomials have the property that their value at $z = \pm 1$ are either equal (for even polynomials), or opposite (for odd ones). Moreover, we can set the value of each of the $P_j(1) = A$ by appropriate, independent (in j) choice of normalization.

The next term is zero:

$$\int_{-1}^{1} P'_{j-1}\, P_j\, dz = 0, \tag{22.36}$$

since any polynomial can be written as a sum of Legendre polynomials up to the same degree, we know that

$$P'_{j-1} = \sum_{k=0}^{j-2} A_k\, P_k, \tag{22.37}$$

and then we know that the dot product of P_j with each of the terms in the sum is zero (from above).

Putting it together, we have:

$$A^2 = \left(j + \frac{1}{2}\right) \int_{-1}^{1} P_j^2\, dz \longrightarrow \frac{A^2}{j + \frac{1}{2}} = \int_{-1}^{1} P_j^2\, dz. \tag{22.38}$$

Taking $A = 1$[1], the usual normalization follows, and our final orthonormality condition reads:

$$P_j \cdot P_k = \frac{2}{j + 2}\, \delta_{jk}. \tag{22.39}$$

22.6 Associated Legendre Polynomials

Now let's return to the full problem (22.5), with our identification $z = \cos\theta$, we have:

$$\left(1 - z^2\right) \frac{d}{dz}\left((1 - z^2) g'\right) + \left[(1 - z^2)\, \ell\, (\ell + 1) - m^2\right] g = 0. \tag{22.40}$$

Suppose we let $g(z) = (1 - z^2)^{m/2} f(z)$ in the above, then

$$\left(1 - z^2\right) f''(z) - 2\,(m + 1)\; z\, f'(z) + \left(\ell\,(\ell + 1) - m\,(m + 1)\right)\; f(z) = 0. \tag{22.41}$$

[1]Think of the even solutions in (22.18) – if we require $P_0(1) = 1$, then $\alpha_0 = 1$. If we want $P_2(1) = 1$, then we set $\alpha_0 = -\frac{1}{2}$. For $P_4(1) = 1$, we need $\alpha_0 = \frac{3}{8}$. These are the coefficients found in, for example Table 4.1 of Griffiths.

Set $m = 0$, and we have Legendre's equation with solution $P_\ell(z)$. If we differentiate the above w.r.t. z, we get

$$\left(1 - z^2\right) \left(\frac{df}{dz}\right)'' - 2\left((m+1)+1\right) z \left(\frac{df}{dz}\right)' + \left(\ell\,(\ell+1) - (m+1)\,(m+2)\right) \left(\frac{df}{dz}\right) = 0. \tag{22.42}$$

Now we can see that this is (22.41) with $m \to m+1$, and $f(z) \to f'(z)$. So if $P_\ell(z)$ solves (22.41) with $m = 0$ (as we know it does, since this is Legendre's equation), then $P'_\ell(z)$ solves (22.41) with $m = 1$. The process continues, if we differentiate again, $P''_\ell(z)$ solves (22.41) with $m = 2$.

In general, then, the function:

$$P_\ell^m(z) = \left(1 - z^2\right)^{m/2} \frac{d^m}{dz^m} P_\ell(z) \tag{22.43}$$

solves (22.40). These are called the "associated Legendre polynomials". Notice that for integer ℓ, we can have m either positive or negative, and it "must be" an integer. In addition, these polynomials will vanish for $|m| > \ell$ since in that case, we have differentiated x^0 w.r.t. x.

22.7 Harmonic Oscillator in One Dimension

Recall the time-independent Schrödinger equation for the harmonic oscillator in one dimension:

$$-\frac{\hbar^2}{2\,m}\,\psi''(x) + \frac{1}{2}\,m\,\omega^2\,x^2\,\psi(x) = E\,\psi(x). \tag{22.44}$$

We want to solve this equation using a series approach.

22.7.1 Step 1

Let's rewrite the equation in a spatially unitless form (the advantage here, aside from cleaning up the various constants that appear, is that we can then compare our unitless quantity to other unitless quantities). If we write the above as:

$$\psi'' - \frac{m^2\,\omega^2}{\hbar^2}\,x^2\,\psi = -\frac{2\,m\,E}{\hbar^2}\,\psi, \tag{22.45}$$

then it is clear, since each term must have units of $\frac{|\psi|}{L^2}$ (look at the first term, for example), that

$$\left|\frac{m^2\,\omega^2}{\hbar^2}\right| = L^{-4}. \tag{22.46}$$

Define the unitless quantity (meant to replace x):

$$\bar{x} = \sqrt{\frac{m\,\omega}{\hbar}}\,x, \tag{22.47}$$

then

$$\frac{1}{\frac{\hbar}{m\,\omega}}\,\frac{\partial^2\psi(\bar{x})}{\partial\bar{x}^2} - \frac{m^2\,\omega^2}{\hbar^2}\,\frac{\hbar}{m\,\omega}\,\bar{x}^2\,\psi(\bar{x}) = -\frac{2\,m\,E}{\hbar^2}\,\psi(\bar{x}). \tag{22.48}$$

Finally, we can multiply to get (understanding ψ as a function of $\bar{x}$, now):

$$\psi'' - \bar{x}^2\,\psi = -\underbrace{\frac{2\,E}{\hbar\,\omega}}_{\equiv\alpha}\,\psi, \tag{22.49}$$

and each term in this expression has the units of ψ only.

22.7.2 Step 2

Next, we take our equation:

$$\psi'' - \left(\bar{x}^2 - \alpha\right)\,\psi = 0 \tag{22.50}$$

and introduce the desired behavior at spatial infinity. If we take $\bar{x} \gg \alpha$ (see the advantage of unitless $\bar{x}$?), then

$$\psi''(\bar{x}) \sim \bar{x}^2\,\psi \longrightarrow \psi \sim e^{\pm\frac{1}{2}\,\bar{x}^2}, \tag{22.51}$$

where we are only approximating the behavior at spatial infinity – this is, however, what we expect. The danger is that we will pick up the growing exponential, so we make an ansatz:

$$\psi(\bar{x}) = e^{-\frac{1}{2}\,\bar{x}^2}\,\bar{\psi}(\bar{x}). \tag{22.52}$$

There is nothing lost in making this initial guess, it is only *motivated* by the desired behavior at spatial infinity.

We rewrite our scaled (22.50) in terms of $\bar{\psi}$ by noting:

$$\begin{aligned}\psi' &= -\bar{x}\, e^{-\frac{1}{2}\bar{x}^2}\, \bar{\psi} + e^{-\frac{1}{2}\bar{x}^2}\, \bar{\psi}' \\ \psi'' &= -e^{-\frac{1}{2}\bar{x}^2}\, \bar{\psi} + \bar{x}^2\, e^{-\frac{1}{2}\bar{x}^2} - 2\,\bar{x}\, e^{-\frac{1}{2}\bar{x}^2}\, \bar{\psi}' + e^{-\frac{1}{2}\bar{x}^2}\, \bar{\psi}''\end{aligned} \tag{22.53}$$

and inputting in (22.50), we have:

$$\boxed{\bar{\psi}'' - 2\,\bar{x}\,\bar{\psi}' + (\alpha - 1)\;\bar{\psi} = 0}. \tag{22.54}$$

22.7.3 Step 3

We are ready to make the series expansion ansatz and input into the final form (22.54). We will, of course, be making the expansion in $\bar{x}$ for the function $\bar{\psi}(\bar{x})$. In order to cover general series, which may not have leading term $\bar{x}^0$, we introduce a factor of $\bar{x}^p$ in front of the infinite sum, allowing our series to start with $\bar{x}^p$ – p must be determined in the process of solving (22.54). Take

$$\bar{\psi}(\bar{x}) = \bar{x}^p \sum_{j=0}^{\infty} a_j\, \bar{x}^j = \sum_{j=0}^{\infty} a_j\, \bar{x}^{j+p}. \tag{22.55}$$

We need the first and second derivatives, and it's easiest to tabulate all the ingredients before putting them into the ODE, so

$$\begin{aligned}\bar{\psi}' &= \sum_{j=0}^{\infty} a_j\,(j+p)\;\bar{x}^{j+p-1} \\ \bar{x}\,\bar{\psi}' &= \sum_{j=0}^{\infty} a_j\,(j+p)\;\bar{x}^{j+p} \\ \bar{\psi}'' &= \sum_{j=0}^{\infty} a_j\,(j+p)\,(j+p-1)\;\bar{x}^{j+p-2}.\end{aligned} \tag{22.56}$$

In order to combine terms, we pull an overall factor of $\bar{x}^p$ out,

$$\bar{x}^p \left[\sum_{j=0}^{\infty} a_j\,(j+p)\,(j+p-1)\;\bar{x}^{j-2} + \sum_{j=0}^{\infty} a_j\,(-2\,(j+p) + (\alpha-1))\;\bar{x}^j\right] = 0. \tag{22.57}$$

The first term, coming from the second derivative, is not written in terms of $\bar{x}^j$ – remember, the idea behind the Frobenius method is to kill each power of $\bar{x}$ in the infinite sum separately. But we can rewrite the offending term by setting $q = j - 2$, to get

$$\begin{aligned}\sum_{j=0}^{\infty} a_j\,(j+p)\,(j+p-1)\;\bar{x}^{j-2} &= \sum_{q=-2}^{\infty} a_{q+2}\,(p+q+2)\,(p+q+1)\;\bar{x}^{q} \\ &= a_0\,p\,(p-1)\;\bar{x}^{-2} + a_1\,(p+1)\;p\,\bar{x}^{-1} \\ &\quad+ \sum_{q=0}^{\infty} a_{q+2}\,(p+q+2)\,(p+q+1)\;\bar{x}^{q}\end{aligned} \tag{22.58}$$

and then rellabeling the dummy index $q \to j$, we can combine with the rest of the terms in the sum:

$$\begin{aligned}0 &= a_0\,p\,(p-1)\;\bar{x}^{-2} + a_1\,(p+1)\;p\,\bar{x}^{-1} \\ &+ \sum_{j=0}^{\infty}\left[a_{j+2}\,(p+j+2)\,(p+j+1) - a_j\,(2\,(p+j) - (\alpha-1))\right]\;\bar{x}^{j}.\end{aligned} \tag{22.59}$$

In order to get rid of the first two terms, we can set $p = 0$, and this leaves us free to choose a_0 and a_1. Then we have the recursion relation implied by the requirement that the coefficient of $\bar{x}^j$ be zero:

$$a_{j+2} = \frac{2\,j + 1 - \alpha}{(j+1)\,(j+2)}\,a_j. \tag{22.60}$$

From the recursion relation, it is clear that setting $a_0 = 0$, we get an odd series, and for $a_1 = 0$, we get an even series.

What is the asymptotic behavior of this recursion relation? For large j, we have $a_{j+2} \sim \frac{2}{j}\,a_j$. If we think about series that have a relation of this type as their recursion, with a factor of z^2 between successive terms, the natural one that comes to mind is:

$$e^{z^2} = \sum_{j=0}^{\infty} \frac{1}{j!}\,z^{2\,j} \tag{22.61}$$

and the coefficient for the $z^{2\,j}$ term is $c_j = \frac{1}{j!}$, while for the $z^{2\,(j-1)}$ term, it is $c_{j-1} = \frac{1}{(j-1)!}$, giving:

$$\frac{c_j}{c_{j-1}} = \frac{1}{j}. \tag{22.62}$$

So our series goes, asymptotically, like $e^{\bar{x}^2}$. That will not give a normalizable solution when combined in the full wavefunction $\psi(x) = e^{-\frac{1}{2}\,\bar{x}^2}\,\bar{\psi}$. In order to maintain normalizability, we must *truncate* the series. There must be some J for which $a_{J+2} = 0$ (and then all the higher coefficients will automatically vanish). This leaves us with a finite set of terms, i.e. a polynomial in $\bar{x}$.

The requirement, for truncation is that:

$$2\,J + 1 = \alpha \equiv \frac{2\,E}{\hbar\,\omega} \longrightarrow E_J = \hbar\,\omega\left(\frac{1}{2} + J\right). \tag{22.63}$$

This is precisely the spectrum we got from our ladder approach. The polynomials associated with the recursion relation above are called "Hermite polynomials" and denoted $H_J(x)$. With the appropriate normalization, the wave function is:

$$\boxed{\psi_J(\bar{x}) = \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^J\,J!}}\,H_J(\bar{x})\,e^{-\frac{1}{2}\,\bar{x}^2},} \tag{22.64}$$

with energy

$$\boxed{E_J = \left(J + \frac{1}{2}\right)\,\hbar\,\omega.} \tag{22.65}$$

Homework

Reading: Griffiths, pp. 51–57 (for harmonic oscillator series expansion).

Griffiths, pp. 133–139 (for spherical separation-of-variables).

Problem 22.1

In this problem, we will work through the Frobenius method for a . . . particular potential. The ultimate goal is the set of discrete energies, not the series solution itself. Our starting point will be the separated radial wave equation.

a. From separation of variables applied to the time-independent Schrödinger equation, we have

$$\frac{1}{f(r)}\frac{d}{dr}\left(r^2\,\frac{df(r)}{dr}\right)-\frac{2\,m\,r^2}{\hbar^2}\,\left[V(r)-E\right]=\ell\,(\ell+1) \tag{22.66}$$

for integer ℓ. Transform to the new function $u(r)\equiv r\,f(r)$, and show that the above can be written as:

$$\frac{d^2u(r)}{dr^2}-\left[\frac{2\,m}{\hbar^2}\,(V(r)-E)+\frac{\ell\,(\ell+1)}{r^2}\right]u(r)=0 \tag{22.67}$$

b. Set

$$V(r)=-\frac{\beta}{r} \tag{22.68}$$

where β (>0) has units $|\beta|=M\,L^3\,T^{-2}$ (where M is mass, L is length, T is time). Inputting this into (22.67), identify a unitless quantity to replace r – that is, find $z=A\,r$ where z is unitless, and A is some combination of constants provided by the problem (i.e. $\hbar$, m, β, etc.).

Rewrite your equation in terms of this new variable z, and define $\alpha^2=-B\,E$, where B is whatever mess of coefficients appears in front of E in your equation. The point here is that we expect $E<0$, and we don't want to carry around a bunch of factors that might hinder the calculation.

c. Now we want to isolate the large z solution, and ensure that we can obtain normalizable wavefunctions. Solve your equation from part b. for z

very large (first reduce your equation by assuming z is large, then solve). Choose the solution (there should be two) that will vanish at spatial infinity, and call it $G(z)$.

d. Next define $u(z) = \bar{u}(z)\, G(z)$. Find the ODE that $\bar{u}(z)$ must satisfy by inserting this form into your equation from Part b. You should end up with:

$$\bar{u}'' - 2\,\alpha\,\bar{u}' + \left(\frac{2}{z} - \frac{\ell\,(\ell+1)}{z^2}\right)\bar{u} = 0. \tag{22.69}$$

e. Finally, the series expansion: Set

$$\bar{u}(z) = z^p \sum_{j=0}^{\infty} a_j\, z^j, \tag{22.70}$$

calculate all relevant derivatives and insert this into your equation from part d. Write the recursion relation for the various coefficients, and the "indicial" equation governing the choice of p. Note that you should get two possible values for p, but one can be dropped based on bad behavior at $z = 0$.

f. For the valid choice of p, write your recursion relation in the form $a_{j+1} = Z\, a_j$ (where Z is some combination of p and j and/or constants) and assume it must truncate at some maximum value J. For this maximum value, we will have $a_{J+1} = 0$ – use this to solve for α, and then find the energy E (related to α from part b.) for this quantum system governed by a potential of the form $-\frac{\beta}{r}$ – your answer should be indexed by an integer, the allowed energies for the stationary states.

Note: The necessity of truncation of the series you have developed is based on the asymptotic behavior of its coefficients – we will discuss this in detail in class.