Orthogonal Polynomials Used in Quantum Mechanics

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1 Preliminaries

This course has a propensity for using special functions and polynomials: it so happens that many of the classically studied sets of orthogonal polynomials feature in bound states of the Schrödinger equation for certain common potentials. We give here derivations of their various properties. The first section is an introduction, the second covers the Hermite polynomials and the harmonic oscillator, the third the Legendre polynomials, the fourth the spherical harmonics in three dimensions, and the fifth the Laguerre polynomials and the hydrogen atom. The last page has a table of the important properties and a list of the first few of each type.

Notational note We will write $D = d/dx$ throughout this handout, both to save space and make it easier to think of it as an operator. In particular, we then have $[x, D] = -1$, and the important result known as *Leibniz's rule*:

$$D^n fg = \sum_{k=0}^{n} \binom{n}{k} (D^k f)(D^{n-k} g).$$

We recall that:

- A *Sturm–Liouville equation* on the interval (a, b) is one in the form
$$-DpDu + qu = \lambda wu, \tag{1}$$
with conditions so that $u \to 0$ at the endpoints or $u' \to 0$ at the endpoints.
- $p > 0$ is the integrating factor, the constant λ is called the *eigenvalue*, $w > 0$ is the *weight function*.
- u is the solution, or the *eigenfunction*: we normally impose that $\int u^2 w < \infty$. If this integral is 1, the eigenfunction is said to be normalised, and we write it as $e_{\lambda,n}$ (since there may be more than one with the same eigenvalue).
- The Sturm–Liouville operator $-DpD + q$ is a self-adjoint operator. Therefore we have the usual trio:
  1. The eigenvalues λ are real,
  2. Eigenfunctions with different eigenvalues are orthogonal, with respect to the inner product
  $$(u, v) = \int_a^b \bar{u} v w.$$
  3. We have *Bessel's inequality*,
  $$(f, f) \geqslant \sum_{\lambda,n} \left|(e_{\lambda,n}, u)\right|^2,$$
  where $e_{\lambda,n}$ are the normalised eigenfunctions with eigenvalue λ. If there are enough eigenfunctions to span the space of square-integrable functions, this is actually an equality.

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1.1 Orthogonal Polynomials

Here we give a list of things it is useful to know about orthogonal polynomials. A set of polynomials is *orthogonal* with respect to an inner product if $(P_n, P_m) = 0$ for $m \neq n$.

The orthogonal polynomials we meet in this course are a subset of the so-called *classical* orthogonal polynomials, which conventionally includes Hermite, Laguerre, Legendre, Gegenbauer/ultraspherical, Jacobi, and Chebyshev.[1,2] They arise as the solutions of certain Sturm–Liouville problems, most of which happen to come up in basic quantum mechanical systems. In this section, P_n are orthogonal polynomials satisfying a differential equation $-DpDP_n = \lambda_n w P_n$ on the interval $[a, b]$: this encompasses all the cases we consider subsequently. Here, the inner product is the Sturm–Liouville one, $(u, v) = \int_a^b uvw$.

1. The *Rodrigues formula* is often the simplest way of defining the polynomials. In the classical cases, it is given by

$$P_n(x) = \frac{1}{\kappa_n w(x)} D^n \left(w(x)(p(x)/w(x))^n \right). \tag{2}$$

   The values of κ_n are chosen so the polynomials satisfy a certain scale convention: for example, the Hermite and Laguerre polynomials conventionally have leading coefficients 2^n and $(-1)^n/n!$ respectively, whereas the Legendre polynomials are set up so that $P_\ell(1) = 1$.

2. Various *recurrence relations* exist relating P_n, normally relating it or its derivative to other polynomials. The central one of these is the *three-term recurrence*, which is always in the form

$$P_{n+1}(x) + (a_n x + b_n)P_n(x) + c_n P_{n-1}(x) = 0. \tag{3}$$

   (This is fairly straightforward to see using orthogonality and that multiplication by x is a self-adjoint operator.)

3. The *generating function* of a set of polynomials is an alternative to the Rodrigues formula for obtaining explicit forms and recurrence relations. It is a function of the form

$$G_P(t, x) = \sum_{n=0}^{\infty} t^n P_n(x) \quad \text{or} \quad g_P(t, x) = \sum_{n=0}^{\infty} \frac{t^n}{n!} P_n(x)$$

   (the former is an *ordinary* generating function, the latter an *exponential* generating function; which one is more useful depends on the situation). The advantage of a generating function is that it tends to be easier to work with and derive properties from; this comes at the price of being much more difficult to find in the first place. Indeed, we normally have to use the three-term recurrence to obtain it.

For proofs of the above general facts, I recommend consulting the following.

- The Wikipedia article on `http://en.wikipedia.org/wiki/Classical_orthogonal_polynomials` ,which is a good summary.
- Roelof Koekoek has some nice notes, with proofs, about orthogonal polynomials on this page: `http://homepage.tudelft.nl/11r49/onderw1617/specfunc_en.html` .

[1] You have actually already met the Chebyshev polynomials: they are defined by $T_n(\cos\theta) = \cos n\theta$ and $U_n(\cos\theta) = \sin(n+1)\theta/\sin\theta$.

[2] The Legendre polynomials are special cases of the Gegenbauer polynomials, which in turn are special cases of the Jacobi polynomials. "Ultraspherical", because you can use the Gegenbauer polynomials as eigenfunctions of the axisymmetric angular Laplacian in n dimensions, in the same way as the Legendre polynomials in 3 dimensions.

2 Hermite Polynomials

Differential Equation The Hermite differential equation is

$$u'' - 2xu' + 2\lambda u = 0. \tag{4}$$

This is a second-order differential equation with analytic coefficients, and is in general not solvable in terms of elementary functions. If we use the Method of Frobenius to find a series expansion $u = \sum_{n=0}^{\infty} a_n x^n$ about $x = 0$, we find the recurrence relation

$$a_{n+2} = \frac{2(n-\lambda)}{(n+1)(n+2)} a_n. \tag{5}$$

Therefore there are two linearly independent solutions, an odd one and an even one. Further, there is a polynomial solution if and only if one of the series terminates, which means that we need $\lambda = N$ for some nonnegative integer N. These polynomial solutions are normally labelled $H_0, H_1, \dots$, and are called the *Hermite polynomials.*

Putting (4) in Sturm–Liouville form, we have

$$-(e^{-x^2} u')' = 2\lambda e^{-x^2} u. \tag{6}$$

Applying the results of Sturm–Liouville theory, we then see that the Hermite polynomials are orthogonal polynomials on $(-\infty, \infty)$ with weight e^{-x^2}, so we have

$$\int_{-\infty}^{\infty} H_m(x) H_n(x) e^{-x^2} \, dx = 0 \qquad \text{if } m \neq n.$$

There is also the question of normalisation. It is conventional, as with many other orthogonal polynomials, to work with functions that are normalised in a different way from $(f, f) = 1$: in this case, the standard definition takes the leading coefficient as 2^n, as we will see below.

Rodrigues Formula The Hermite polynomials are most easily defined using the Rodrigues formula

$$H_n(x) = (-1)^n e^{x^2} D^n e^{-x^2}, \tag{7}$$

from which we can obtain

Recurrence Relations Firstly, by using Leibniz's rule we have

$$H_{n+1}(x) = (-1)^n e^{x^2} D^n(-De^{-x^2}) = (-1)^n e^{x^2} D^n(2xe^{-x^2}) = 2xH_n(x) - 2nH_{n-1}, \tag{8}$$

the three-term recurrence relation. From this and $H_0(x) = 1$, $H_1(x) = 2x$ it follows that in the conventional definition, the leading coefficient in $H_n(x)$ is 2^n. On the other hand, separating a derivative from the other side of D^{n+1},

$$H_{n+1}(x) = -e^{x^2} De^{-x^2} H_n(x) = 2xH_n(x) - H_n'(x).$$

Equating this to the other expression for H_{n+1}, $H_n'(x) = 2nH_{n-1}(x)$. Differentiating the previous equation gives

$$H_n''(x) - 2H_n(x) - 2xH_n'(x) = -H_{n+1}'(x) = -2(n+1)H_n(x),$$

which implies that H_n does satisfy (4). As for orthogonality, we use lots of integration by parts and discarding of the vanishing boundary terms to find that

$$\int_0^{\infty} H_m(x) H_n(x) e^{-x^2} \, dx = (-1)^n \int_0^{\infty} H_m(x) D^n e^{-x^2} \, dx = \int_0^{\infty} [D^n H_m(x)] e^{-x^2} \, dx$$

This is zero if $n > m$ since H_m has degree m. By symmetry, it is also zero if $n < m$, and if $n = m$, only the leading term remains, and so we find that

$$\int_0^{\infty} H_m(x) H_n(x) e^{-x^2} \, dx = 2^n n! \sqrt{\pi} \delta_{mn}. \tag{9}$$

Generating Function The Hermite polynomials have exponential generating function

$$g_H(t,x) = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(x) = e^{2xt-t^2}, \tag{10}$$

which may be found by substituting g_H into (8), which becomes $g_H' + 2(t-x)g_H = 0$; this is then simple to solve.

2.1 Application: Harmonic Oscillator

The time-independent Schrödinger equation for the harmonic oscillator is

$$-\frac{\hbar^2}{2m}\psi'' + \frac{m\omega^2}{2}x^2\psi = E\psi. \tag{11}$$

Setting $y = \sqrt{m\omega/\hbar}x$ and $\mathcal{E} = 2E/(\hbar\omega)$, this equation becomes the non-dimensional equation

$$-\psi'' + (y^2 - \mathcal{E})\psi = 0. \tag{12}$$

The large-y behaviour is determined by the y^2, and we guess[3] that $\psi(y) \sim e^{-y^2/2}$ as $y \to \pm\infty$. Therefore we look for solutions in the form

$$\psi(y) = u(y)e^{-y^2/2}.$$

Substituting this into the non-dimensional differential equation gives

$$u'' - 2yu' + (\mathcal{E} - 1)u = 0,$$

which is the Hermite equation (4) if $\mathcal{E} = 2\lambda + 1$. One can check using the large-n asymptotics of (5) that any non-polynomial solution to this equation grows like e^{y^2}, so to be normalisable, we must have a polynomial solution. Therefore we must have $\mathcal{E} = 2N+1$, and then the normalised solution to (12) with this energy is $\frac{1}{2^{N/2}\sqrt{N!}}H_N(y)e^{-y^2/2}$.

3 Legendre Polynomials and Associates

Differential Equation The Legendre equation is

$$-((1-x^2)u')' = \ell(\ell+1)u. \tag{13}$$

It is a Sturm–Liouville equation on the interval $[-1,1]$, and we are interested in the *continuous* solutions. $x = 0$ is a regular point, and using the Method of Frobenius gives the recurrence relation

$$a_{n+2} = \frac{(n-\ell)(n+\ell+1)}{(n+1)(n+2)}a_n. \tag{14}$$

For large enough n, the coefficients have the same sign, and for large n, the ratio of successive coefficients tends to 1; hence the series blows up at $x = 1$,[4] so we need it to terminate to obtain a continuous solution. Hence ℓ is a nonnegative integer, in which case there is a polynomial solution of degree ℓ, which is called a *Legendre polynomial*, $P_\ell(x)$. Sturm–Liouville theory implies that these polynomials are orthogonal on $[-1,1]$ with weight 1:

$$\int_{-1}^{1} P_\ell(x)P_{\ell'}(x)\,dx = 0 \qquad \text{if } \ell \neq \ell'.$$

Rodrigues Formula P_ℓ may be defined using the (original) Rodrigues formula,

$$P_\ell(x) = \frac{1}{2^\ell \ell!}D^\ell(x^2-1)^\ell. \tag{15}$$

Since the interior function changes with ℓ, this is much harder to work with than the one for the Hermite polynomials.

[3]See Asymptotic Methods next year for where this comes from.

[4]It has to blow up somewhere on the unit circle, and the large-n coefficients having the same sign forces this to occur on the positive real axis.

Recurrence relations By differentiating in two different ways, we have the following two relationships:

$$D^{a+1}(x^2-1)^{b+1} = a(a+1)D^{a-1}(x^2-1)^b + 2(a+1)xD^a(x^2-1)^b + (x^2-1)D^{a+1}(x^2-1)^b \tag{16}$$

$$\begin{aligned} D^{c+1}(x^2-1)^{d+1} &= 2(d+1)D^c x(x^2-1)^d \\ &= 2c(d+1)D^{c-1}(x^2-1)^d + 2(d+1)xD^c(x^2-1)^d \end{aligned} \tag{17}$$

Taking $c = \ell+1$, $d = \ell$ in the second, we have

$$\begin{aligned} D^{\ell+2}(x^2-1)^{\ell+1} &= 2(\ell+1)^2 D^\ell(x^2-1)^\ell + 2(\ell+1)xD^{\ell+1}(x^2-1)^\ell \\ DP_{\ell+1}(x) &= (\ell+1)P_\ell(x) + xDP_\ell(x), \end{aligned} \tag{18}$$

dividing by $2^{\ell+1}(\ell+1)!$. Taking $a = \ell+1$, $b = \ell$ in the first gives

$$\begin{aligned} D^{\ell+2}(x^2-1)^{\ell+1} &= (\ell+1)(\ell+2)D^\ell(x^2-1)^\ell + 2(\ell+2)xD^{\ell+1}(x^2-1)^\ell + (x^2-1)D^{\ell+2}(x^2-1)^\ell \\ 2(\ell+1)DP_{\ell+1}(x) &= (\ell+1)(\ell+2)P_\ell(x) + 2(\ell+2)xDP_\ell(x) + (x^2-1)D^2P_\ell(x) \end{aligned}$$

Substituting for $DP_{\ell+1}(x)$ using (18) gives

$$(x^2-1)D^2P_\ell(x) + 2xDP_\ell(x) - \ell(\ell+1)P_\ell(x) = 0,$$

which proves that P_ℓ is a solution to the Legendre equation (13) with eigenvalue $\ell(\ell+1)$.

We can get more out of such identities, however: if we put $a = b = c = d = \ell$, then the identities become

$$\begin{aligned} D^{\ell+1}(x^2-1)^{\ell+1} &= \ell(\ell+1)D^{\ell-1}(x^2-1)^\ell + 2(\ell+1)xD^\ell(x^2-1)^\ell + (x^2-1)D^\ell(x^2-1)^{\ell-1} \\ D^{\ell+1}(x^2-1)^{\ell+1} &= 2\ell(\ell+1)D^{\ell-1}(x^2-1)^\ell + 2(\ell+1)xD^\ell(x^2-1)^\ell \end{aligned}$$

but the $D^{\ell-1}(x^2-1)^\ell$ terms don't have a nice interpretation. This doesn't actually matter, since we can eliminate them between the equations by subtracting the second from twice the first, which gives

$$\begin{aligned} D^{\ell+1}(x^2-1)^{\ell+1} &= 2(\ell+1)xD^\ell(x^2-1)^\ell + 2(x^2-1)D^\ell(x^2-1)^{\ell-1} \\ (\ell+1)P_{\ell+1}(x) &= (\ell+1)xP_\ell(x) + (x^2-1)DP_\ell(x). \end{aligned} \tag{19}$$

Writing down another copy of this identity with ℓ replaced by $\ell-1$ and applying (18), we have

$$\begin{aligned} \ell P_\ell(x) - \ell xP_{\ell-1}(x) &= (x^2-1)DP_{\ell-1}(x) \\ &= \frac{(x^2-1)DP_\ell(x) - (x^2-1)\ell P_{\ell-1}(x)}{x} \\ &= \frac{(\ell+1)P_{\ell+1}(x) - (\ell+1)xP_\ell(x) - (x^2-1)\ell P_{\ell-1}(x)}{x} \end{aligned}$$

using (19). Rearranging this gives the three-term recurrence

$$(\ell+1)P_{\ell+1}(x) - (2\ell+1)xP_\ell(x) + \ell P_{\ell-1}(x) = 0. \tag{20}$$

One can obtain other similar identities, but this is plenty for our purposes.

Generating Function As may be apparent, this Rodrigues formula is not very easy to work with. Our life is much improved if we use the generating function,

$$G_P(t,x) = \sum_{\ell=0}^{\infty} t^\ell P_\ell(x) = \frac{1}{\sqrt{1+t^2-2tx}}. \tag{21}$$

To find this, we substitute into the three-term recurrence relation, which gives the equation $G_P' - (2tG_P' + G_P)x + (t^2G_P' + tG_P) = 0$, or $(t-x)G_P + (1+t^2-2tx)G_P' = 0$, which gives the result in (21). In particular, with this it is obvious that $P_\ell(1) = 1$, which would otherwise have been a right pain to prove. Another quick application of this result gives us the normalisation: since we know that $(P_\ell, P_{\ell'}) = 0$ if $\ell \neq \ell'$, we have

$$(G_P(t), G_P(t)) = \sum_{\ell,\ell'=0}^{\infty} t^{\ell+\ell'}(P_\ell, P_{\ell'}) = \sum_{\ell,\ell'=0}^{\infty} t^{\ell+\ell'}(P_\ell, P_\ell)\delta_{\ell\ell'} = \sum_{\ell=0}^{\infty} t^{2\ell}(P_\ell, P_\ell),$$

from which we can read off the values of the normalisation constants. In this case,

$$\begin{aligned}(G_P(t), G_P(t)) &= \int_{-1}^{1} \frac{dx}{1 + t^2 - 2tx} \\ &= -\frac{1}{2t}\left(\log\left(1 + t^2 - 2t\right) - \log\left(1 + t^2 + 2t\right)\right) \\ &= \frac{1}{t}\log\left(\frac{1+t}{1-t}\right) \\ &= \sum_{\ell=0}^{\infty} t^{2\ell}\frac{2}{2\ell+1},\end{aligned}$$

so

$$\int_{-1}^{1} P_\ell(x)P_{\ell'}(x)\,dx = \frac{2}{2\ell+1}\delta_{\ell\ell'}. \tag{22}$$

3.1 Associated Legendre equation

Differentiating (13) m times gives

$$-(1 - x^2)(u^{(m)})'' + 2x(m+1)(u^{(m)})' + m(m+1)u^{(m)} = \ell(\ell+1)u^{(m)}$$

and then substituting $u^{(m)} = (1 - x^2)^{-m/2}v$ gives, after a struggle, the *associated Legendre equation*,

$$-\left((1 - x^2)v'\right)' + \frac{m^2}{1 - x^2}v = \ell(\ell+1)v. \tag{23}$$

Unwinding this process, we conclude that if m is an integer, this equation has solutions

$$P_\ell^m(x) = (-1)^m(1 - x^2)^{m/2}D^m P_\ell(x) = \frac{(-1)^m}{2^\ell \ell!}(1 - x^2)^{m/2}D^{m+\ell}(x^2 - 1)^\ell, \tag{24}$$

which are sometimes called the *associated Legendre polynomials*, even though if m is odd they aren't actually polynomials.[5] The first definition makes sense for $0 \leqslant m$, but the second can be used to extend it to $m \geqslant -\ell$. In order for this solution to be nontrivial, we need $-\ell \leqslant m \leqslant \ell$: this is clear for $m > \ell$. We can verify the other end indirectly: we show that P_ℓ^m and P_ℓ^{-m} are proportional.

Sturm–Liouville theory tells us again the P_ℓ^m are orthogonal (for different ℓ) with weight 1. Moreover, they are also orthogonal for different m, with weight $(1 - x^2)^{-1}$. The equation is unchanged on replacing m by $-m$, so both P_ℓ^m and P_ℓ^{-m} satisfy it. Lastly, there is only one linearly independent solution to the equation that is finite at $x = 0$, so $P_\ell^{-m} = c_{\ell m}P_\ell^m$ for some $c_{\ell m}$. All this theory means that we just have to check the leading coefficient on both sides of

$$D^{\ell-m}(x^2 - 1)^\ell = c_{\ell m}(1 - x^2)^m D^{\ell+m}(x^2 - 1)^\ell;$$

this gives

$$P_\ell^{-m}(x) = (-1)^m\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(x). \tag{25}$$

Therefore we take $-\ell \leqslant m \leqslant \ell$, to avoid problems with factorials of negative numbers.

Essentially any recurrence that the Legendre polynomials have generalises into one for the associated Legendre polynomials in the obvious way (i.e. differentiate m times and multiply as necessary). The orthogonality with respect

[5] The $(-1)^m$, called the Condon–Shortley phase, makes the solutions have nicer properties when used to discuss angular momentum in Principals of Quantum Mechanics next year.

to m generates another set of identities, which can also be obtained by differentiation of the definition. We elide both for reasons of space.

The next question is of normalisation. After applying (25) we can use the result for the ordinary Legendre polynomials:

$$\begin{aligned}\int_{-1}^{1} P_\ell^m(x)P_{\ell'}^m(x)\,dx &= (-1)^m\frac{(\ell+m)!}{(\ell-m)!}\int_{-1}^{1} P_\ell^{-m}(x)P_{\ell'}^m(x)\,dx \\ &= (-1)^m\frac{(\ell+m)!}{(\ell-m)!}\int_{-1}^{1}(1-x^2)^{-m/2}\frac{(-1)^m}{2^\ell \ell!}D^{\ell-m}(x^2-1)^\ell(-1)^m(1-x^2)^{m/2}D^mP_{\ell'}(x)\,dx \\ &= (-1)^m\frac{(\ell+m)!}{(\ell-m)!}\int_{-1}^{1}\frac{1}{2^\ell \ell!}D^{\ell-m}(x^2-1)^\ell D^mP_{\ell'}(x)\,dx \\ &= \frac{(\ell+m)!}{(\ell-m)!}\int_{-1}^{1}\frac{1}{2^\ell \ell!}D^{\ell}(x^2-1)^\ell P_{\ell'}(x)\,dx \\ &= \frac{(\ell+m)!}{(\ell-m)!}\int_{-1}^{1}P_\ell(x)P_{\ell'}(x)\,dx \\ &= \frac{(\ell+m)!}{(\ell-m)!}\frac{2}{2\ell+1}\delta_{\ell\ell'},\end{aligned}$$

integrating by parts lots of times and using (22).

4 Spherical Harmonics

The simultaneous eigenfunctions of the angular part of the Laplacian,

$$-\nabla^2+\frac{1}{r}\partial_r^2 r=\frac{L^2}{\hbar^2},$$

and the "z-angular momentum" $L_3/\hbar$ are called *spherical harmonics*, written as $Y(\theta,\phi)$: they satisfy

$$\hbar^{-2}L^2Y=\ell(\ell+1)Y, \qquad \hbar^{-1}L_3Y=mY.$$

These operators are given in terms of angles by

$$\hbar^{-2}L^2=-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)-\frac{1}{\sin^2\theta}\left(\frac{\partial}{\partial\phi}\right)^2 \qquad \hbar^{-1}L_3=-i\frac{\partial}{\partial\phi}.$$

Therefore we can separate variables as $Y(\theta,\phi)=\Theta(\theta)\Phi(\phi)$, and the equations become

$$-\frac{1}{\sin\theta}\left(\sin\theta\,\Theta'(\theta)\right)'+\frac{m^2}{\sin^2\theta}\Theta(\theta)=\ell(\ell+1)\Theta(\theta) \tag{26}$$

$$-i\Phi'=m\Phi. \tag{27}$$

The Φ equation is easy to solve, and gives $\Phi(\phi)=e^{im\phi}$. m must be an integer for this function to be continuous. The Θ equation looks familiar if we make the change of variables $x=\cos\theta$: then $\frac{d}{dx}=\sin\theta\frac{d}{d\theta}$ so the equation becomes

$$-\left((1-x^2)\Theta'(x)\right)'+\frac{m^2}{1-x^2}\Theta(x)=\ell(\ell+1)\Theta(x),$$

i.e. the associated Legendre equation (23). The spherical harmonics are therefore

$$Y_{\ell,m}(\theta,\phi)=\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}P_\ell^m(\cos\theta)e^{im\phi}, \tag{28}$$

where $\ell\in\{0,1,2,\dots\}$, $m\in\{-\ell,-\ell+1,\dots,\ell\}$, and the normalisation constant has been chosen so that

$$\int_0^{2\pi}\int_0^{\pi}\overline{Y_{\ell,m}(\theta,\phi)}Y_{\ell',m'}(\theta,\phi)\sin\theta\,d\theta\,d\phi=\delta_{\ell\ell'}\delta_{mm'}.$$

4.1 An Alternative Perspective

This was all rather complicated. Is there a simpler way to understand this?[6]

Our separation of variables led us to believe that the natural coordinates to use are sphericals. But what do spherical harmonics look like in Cartesians?

Suppose first we look at *harmonic polynomials*, which, as you might expect, are polynomials which satisfy Laplace's equation. Since $x = r\sin\theta\cos\phi, y = r\sin\theta\sin\phi, z = r\cos\theta$, each term can be written in the form $r^\ell f(\theta,\phi)$, and then

$$-\hbar^2\nabla^2 r^\ell f = -\ell(\ell+1)\hbar^2 r^{\ell-2} f + r^{\ell-2}L^2 f.$$

If we sum over terms of degree ℓ to obtain a *homogeneous* polynomial p of degree ℓ, then $p(x,y,z)$ is harmonic if and only if $Y(\theta,\phi) = r^{-\ell}p(x,y,z)$ satisfies

$$L^2 Y = \hbar^2\ell(\ell+1)Y, \tag{29}$$

i.e. Y is a spherical harmonic with azimuthal quantum number n. Linearity implies that each homogeneous harmonic polynomial of degree n corresponds to such a spherical harmonic, and hence we can obtain all of them in this way.

How many linearly independent degree-ℓ harmonic polynomials are there? There are $(\ell+1)(\ell+2)/2$ monomials in x, y, z of degree ℓ, so a general homogeneous polynomial has this many coefficients. There are $\ell(\ell-1)/2$ monomials of degree $\ell-2$, so a general harmonic polynomial must satisfy this many conditions to make all terms in its Laplacian vanish. The equations are linear, so we find that there are $(\ell+1)(\ell+2)/2 - \ell(\ell-1)/2 = 2\ell+1$ linearly independent solutions, which agrees with our previous answer of how many to expect.

This gives us the eigenfunctions of L^2. What about $L_3 = -i\hbar(x\partial_y - y\partial_x)$? This is a first-order linear operator, that maps the (finite-dimensional) space of homogeneous polynomials of degree ℓ to themselves.[7] It is also Hermitian, and hence has real eigenvalues, and a basis of orthogonal eigenfunctions. But how do we find them?

Complex ideas come to our rescue here: a quick calculation shows that $(x \pm iy)^m$ is an eigenfunction of L_3 with eigenvalue $\pm m\hbar$. The product $(x+iy)(x-iy) = x^2+y^2$ also has eigenvalue zero, so Leibniz's rule allows us to use this as follows: each eigenfunction of L_3 with eigenvalue m may be written as

$$F_{\ell,m}(x,y,z) = (x + \operatorname{sgn}(m)iy)^{|m|} r^{\ell-|m|} p(z/r), \tag{30}$$

where $r = \sqrt{x^2+y^2+z^2}$ as usual, and p is a polynomial of degree $(\ell - |m|)$ that makes $F_{\ell,m}$ a solution to Laplace's equation. Unravelling this produces the associated Legendre equation, as we might expect.

Written this way, the first few spherical harmonics are proportional to:

$m\backslash\ell$	0	1	2	3
3				$(x+iy)^3$
2			$(x+iy)^2$	$z(x+iy)^2$
1		$x+iy$	$z(x+iy)$	$(5z^2-r^2)(x+iy)$
0	1	z	$3z^2-r^2$	$5z^3-3r^2z$
−1		$x-iy$	$z(x-iy)$	$(5z^2-r^2)(x-iy)$
−2			$(x-iy)^2$	$z(x-iy)^2$
−3				$(x-iy)^3$

5 Laguerre Polynomials

Differential equation For a fixed number $\alpha > -1$, the *generalised Laguerre equation* is given by

$$xu'' + (\alpha+1-x)u' + nu = 0. \tag{31}$$

[6] Of course, or I wouldn't have asked the question.
[7] And hence must commute with L^2.

Applying the Method of Frobenius, there is a regular singular point at $x = 0$. We find that the indicial equation is $\sigma(\sigma+\alpha) = 0$, so regular solutions must in general have $\sigma = 0$, and hence are of the form $\sum_{k=0}^{\infty} a_k x^k$. Then we obtain the recurrence relation

$$a_{k+1} = \frac{k-n}{(k+1)(k+\alpha+1)} a_k. \tag{32}$$

If and only if n is a nonnegative integer, we can have a polynomial solution, which is called the *Laguerre polynomial* $L_n^{(\alpha)}$: the usual convention is to take $(-1)^n/n!$ as the leading coefficient.

Rodrigues formula

$$L_n^{(\alpha)}(x) = \frac{1}{n!} x^{-\alpha} e^x D^n x^{n+\alpha} e^{-x} = \frac{1}{n!} x^{-\alpha} (D-1)^n x^{n+\alpha}; \tag{33}$$

the latter of which follows by writing the differential operator as $e^x D e^{-x} = D - 1$. From here one can extract the general closed-form sum

$$L_n^{(\alpha)}(x) = \sum_{k=0}^{n} (-1)^k \binom{n+\alpha}{n-k} \frac{x^k}{k!}.$$

It is a straightforward, if tedious, exercise to check that (33) satisfies (31), which is most helpfully written in the Sturm–Liouville form $[Dxe^{-x}x^{\alpha}D + nx^{\alpha}e^{-x}]y = 0$ for such purposes.

Recurrence Relations One also obtains recurrence relations:

$$\begin{aligned}(n+1)L_{n+1}^{(\alpha)}(x) &= \frac{x^{-\alpha}}{n!}(D-1)^n(D-1)x^{n+\alpha+1} = \frac{x^{-\alpha}}{n!}(D-1)^n((n+\alpha+1)x^{n+\alpha} - x^{n+\alpha+1}) \\ &= (n+\alpha+1)L_n^{(\alpha)}(x) - xL_n^{(\alpha+1)}(x)\end{aligned} \tag{34}$$

and

$$\begin{aligned} xDL_n^{(\alpha)}(x) &= x\frac{1}{n!}Dx^{-\alpha}e^x D^n x^{n+\alpha}e^{-x} = (x-\alpha)L_n^{(\alpha)}(x) + x\frac{1}{n!}x^{-\alpha}e^x D^{n+1}x^{n+\alpha}e^{-x} \\ &= (x-\alpha)L_n^{(\alpha)}(x) + (n+1)L_{n+1}^{(\alpha-1)}(x) \\ &= (x-\alpha)L_n^{(\alpha)}(x) + (n+\alpha)L_n^{(\alpha-1)}(x) - xL_n^{(\alpha)}(x) \\ &= (n+\alpha)L_n^{(\alpha-1)}(x) - \alpha L_n^{(\alpha)}(x)\end{aligned}$$

Unfortunately neither of these are much use by themselves, since we ideally want to keep α the same. We can derive a few more of this sort of flawed relation by being rather more sophisticated with our manipulation of the derivatives: recall that $[x, (D-1)^n] = (D-1)[x, (D-1)^{n-1}] + [x, D-1](D-1)^{n-1} = \cdots = -n(D-1)^n$. Then we have

$$\begin{aligned} DL_n^{(\alpha)}(x) &= n!^{-1}Dx^{-\alpha}(D-1)^n x^{n+\alpha} \\ &= \frac{1}{n!}x^{-\alpha}\left(D - \frac{\alpha}{x}\right)(D-1)^n x^{n+\alpha} \\ &= \frac{1}{n!}x^{-\alpha-1}\left(x(n+\alpha)(D-1)^n - \alpha(D-1)^n x\right)x^{n+\alpha-1} \\ &= \frac{1}{n!}x^{-\alpha-1}\left((n+\alpha)[x,(D-1)^n] + n(D-1)^n x\right)x^{n+\alpha-1} \\ &= \frac{1}{n!}x^{-\alpha-1}\left(-(n+\alpha)n(D-1)^{n-1} + n(D-1)^n x\right)x^{n+\alpha-1} \\ &= \frac{1}{(n-1)!}x^{-\alpha-1}(D-1)^{n-1}\left(-(n+\alpha) + (D-1)x\right)x^{n+\alpha-1} \\ &= -\frac{1}{(n-1)!}x^{-\alpha-1}(D-1)^{n-1}x^{n+\alpha} = -L_{n-1}^{(\alpha+1)}(x).\end{aligned}$$

On the other hand, we also have

$$\begin{aligned}
n!(D-1)L_n^{(\alpha)}(x) &= (D-1)x^{-\alpha}(D-1)^n x^{n+\alpha} \\
&= x^{-\alpha}\left(-\frac{\alpha}{x}(D-1)^n + (D-1)^{n+1}\right)x^{n+\alpha} \\
&= x^{-\alpha-1}\left(-\alpha(D-1)^n + x(D-1)^{n+1}\right)x^{n+\alpha} \\
&= x^{-\alpha-1}\left(-\alpha(D-1)^n + [x,(D-1)^{n+1}] + (D-1)^{n+1}x\right)x^{n+\alpha} \\
&= x^{-\alpha-1}\left(-(n+\alpha)(D-1)^n + (D-1)^n(n+\alpha-x)\right)x^{n+\alpha} \\
&= -x^{-\alpha-1}(D-1)^n x^{n+\alpha+1} = -n!L_n^{(\alpha+1)}(x),
\end{aligned}$$

and hence

$$DL_{n+1}^{(\alpha)}(x) = (D-1)L_n^{(\alpha)}(x).$$

Another relationship involving three functions is

$$\begin{aligned}
L_n^{(\alpha+1)} &= n!^{-1}x^{-\alpha-1}(D-1)^n x x^{n+\alpha} \\
&= n!^{-1}x^{-\alpha-1}([(D-1)^n, x] + x(D-1)^n)x^{n+\alpha} \\
&= n!^{-1}x^{-\alpha-1}(n(D-1)^{n-1} + x(D-1)^n)x^{n+\alpha} \\
&= L_{n-1}^{(\alpha+1)} + L_n^{(\alpha)}
\end{aligned}$$

Substituting for the $(\alpha+1)$ polynomials in here using (34) gives

$$0 = (n+1)L_{n+1}^{(\alpha)}(x) - (2n+\alpha+1-x)L_n^{(\alpha)}(x) + (n+\alpha)L_{n-1}^{(\alpha)}(x), \tag{35}$$

at last the three-term relation.

Orthogonality Laguerre polynomials with the same α are orthogonal on $(0,\infty)$ with weight $x^\alpha e^{-x}$:

$$\int_0^\infty L_m^{(\alpha)}(x)L_n^{(\alpha)}(x)x^\alpha e^{-x}\,dx = \frac{(n+\alpha)!}{n!}\delta_{mn}.$$

We can check this using the Rodrigues formula: suppose WLOG that $n \geqslant m$. Then, integrating by parts,

$$\begin{aligned}
\int_0^\infty L_m^{(\alpha)}(x)L_n^{(\alpha)}(x)x^\alpha e^{-x}\,dx &= \frac{1}{n!}\int_0^\infty L_m^{(\alpha+1)}(x)(D^n x^{n+\alpha}e^{-x})\,dx \\
&= \frac{(-1)^n}{m!}\int_0^\infty x^{n+\alpha}e^{-x}D^n L_m^{(\alpha+1)}(x)\,dx
\end{aligned}$$

If $m > n$, the derivative vanishes identically, so the integral is zero. On the other hand, if $m = n$ only the leading term remains, and this differentiates to $(-1)^n$. Hence the integral is $\int_0^\infty x^{n+\alpha}e^{-x}\,dx = (n+\alpha)!$, either by induction or definition.

Generating Function Substituting into the three-term relation, we solve the differential equation $(x-(1+\alpha)(1-t))G + (1-t)^2G' = 0$ to find the generating function,

$$G_L(t,x) = \sum_{n=0}^\infty t^n L_n^{(\alpha)}(x) = \frac{1}{(1-t)^{\alpha+1}}\exp\left(-\frac{xt}{1-t}\right).$$

5.1 Application: Hydrogen atom

After separating variables in spherical coordinates, the radial Schrödinger equation for the hydrogen atom with angular momentum $\hbar^2\ell(\ell+1)$ is

$$-\frac{\hbar^2}{2\mu}\frac{1}{r}\left(\frac{d}{dr}\right)^2 rR + \left(\frac{\hbar^2\ell(\ell+1)}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r}\right)R = ER$$

It is sensible to non-dimensionalise the equation: the first step is to change variables to $y = r/r_0$, where $r_0 = 4\pi\epsilon_0\hbar^2/(\mu e^2)$, i.e. the Bohr radius. Then the equation becomes

$$-\frac{r_0^2}{r}\left(\frac{d}{dr}\right)^2 rR + \left(\ell(\ell+1)\frac{r_0^2}{r^2} - 2\frac{r_0}{r}\right)R = \frac{2\mu r_0^2 E}{\hbar^2}R$$

$$-\frac{1}{y}\left(\frac{d}{dy}\right)^2 yR + \left(\frac{\ell(\ell+1)}{y^2} - \frac{2}{y}\right)R = -\nu^2 R,$$

where ν is the non-dimensional constant $-2\mu r_0^2 E/\hbar^2$. We choose this sign because for large y, the equation becomes $-R'' \approx -\nu^2 R$, which has normalisable solution $e^{-\nu y}$.

On the other hand, the small-y behaviour is dominated by the $\ell(\ell+1)/y^2$ term, $-(yR)''/y + \ell(\ell+1)R/y^2 \approx 0$, which has solutions y^ℓ and $y^{-\ell-1}$. We choose y^ℓ since it is regular. Both sorts of behaviour are included if we write

$$R(y) = y^\ell e^{-\nu y} f(y),$$

which (eventually) transforms the equation into

$$yf'' + ((2\ell+1) + 1 - 2\nu y)f' + 2(1 - (\ell+1)\nu)f = 0$$

This is obviously almost the generalised Laguerre equation (31), but we need to rescale the variable again: setting $\rho = 2\nu y$ gives

$$\rho f'' + ((2\ell+1) + 1 - \rho)f + 2(\nu^{-1} - \ell - 1)f.$$

This is precisely (31) with $\alpha = 2\ell+1$, and so we need $\nu^{-1} - \ell - 1$ to be a nonnegative integer to have a polynomial solution.[8] After the dust settles, we conclude that the energy eigenfunctions of the hydrogen atom are

$$\psi_{n\ell m}(x) = \sqrt{\left(\frac{2}{nr_0}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}}\rho^\ell L_{n-\ell-1}^{2\ell+1}(\rho)e^{-\rho/2}Y_\ell^m(\theta,\phi), \tag{36}$$

with energies

$$E_N = -\frac{\hbar^2}{2\mu r_0^2(n+\ell)^2} = -\frac{\mu e^4}{32\pi^2\epsilon_0^2\hbar^2}\frac{1}{N^2} \tag{37}$$

There are $\sum_{\ell=0}^{N-1} 2\ell+1 = N^2$ wavefunctions with this energy, since $N \in \{0,1,2,\dots\}$, $\ell \in \{0,1,\dots,N-1\}$ and $m \in \{-\ell,-\ell+1,\dots,\ell\}$.

[8] One can use the recurrence relation of the coefficients to check that any non-polynomial solution is asymptotic to $e^{2\nu y}$, and hence not normalisable.

6 Summary

Table 1: Properties of orthogonal polynomials in this handout. The first row gives the general case as an example.

Polynomial	Parameters	Interval	Differential equation	Weight	Rodrigues formula	Normalisation	Use
Orthogonal polynomial P_n	$n \in \{0, 1, \dots\}$	$[a, b]$	$-(pu')' + qu = \lambda_n w u$	$w(x)$	$\frac{1}{\kappa_n w} D^n w (p/w)^n$	$\int_a^b (P_n)^2 w$	
Hermite H_n	$n \in \{0, 1, \dots\}$	$\mathbb{R}$	$u'' + 2xu = 2nu$	e^{-x^2}	$e^{x^2} D^n e^{-x^2}$	$2^n n!$	Harmonic Oscillator wavefunctions: with $y = \sqrt{m\omega/\hbar}x$, $\psi_n(x) = H_n(y) e^{-y^2/2}/\sqrt{2^n n!}$
Legendre P_ℓ	$\ell \in \{0, 1, \dots\}$	$[-1, 1]$	$-((1-x^2)u')' = \ell(\ell+1)u$	1	$\frac{1}{2^\ell \ell!} D^\ell (x^2-1)^\ell$	$\frac{2}{2\ell+1}$	Axisymmetric solutions of Laplace's equation: $(Ar^\ell + Br^{-\ell-1}) P_\ell(\cos\theta)$
Associated Legendre P_ℓ^m	$\ell \in \{0, 1, \dots\}$, $m \in \{-\ell, -\ell+1, \dots, \ell\}$	$[-1, 1]$	$-((1-x^2)u')' + \frac{m^2}{1-x^2} = \ell(\ell+1)u$	1 (wrt ℓ)	$\frac{(-1)^m}{2^\ell \ell!} D^{\ell+m} (x^2-1)^\ell$	$\frac{(\ell+m)!}{(\ell-m)!} \frac{2}{2\ell+1}$	Spherical Harmonics: $Y_\ell^m(\theta, \phi) \propto P_\ell^m(\cos\theta) e^{m\phi}$
(Generalised) Laguerre $L_n^{(\alpha)}$	$n \in \{0, 1, \dots\}$ $\alpha > -1$	$[0, \infty)$	$-xu'' - (1+\alpha-x)u = nu$	$x^\alpha e^{-x}$	$\frac{1}{n!} e^x x^\alpha D^n x^{n+\alpha} e^{-x}$ or $\frac{1}{n!} x^\alpha (D-1)^n x^{n+\alpha}$	$\frac{(n+\alpha)!}{n!}$	Hydrogen atom wavefunctions: with $\rho = 2(r/n)\mu e^2/(4\pi\epsilon_0\hbar^2)$, $\psi_{n\ell m}(x) \propto \rho^\ell L_{n-\ell-1}^{(2\ell+1)}(\rho) e^{-\rho/2} Y_\ell^m(\theta, \phi)$

The first few polynomials are given by:

Hermite

$$H_0(x) = 1, \qquad H_1(x) = 2x, \qquad H_2(x) = 4x^2 - 2$$

Legendre

$$P_0(x) = 1, \qquad P_1(x) = x, \qquad P_2(x) = \frac{1}{2}(x^2 - 1)$$

Laguerre

$$L_0^{(\alpha)}(x) = 1, \qquad L_1^{(\alpha)}(x) = -x + (1+\alpha), \qquad L_2^{(\alpha)}(x) = \frac{1}{2}x^2 - (\alpha+2)x + \frac{(\alpha+2)(\alpha+1)}{2}$$

Associated Legendre $P_\ell^m(\cos\theta)$, with $c = \cos\theta$ and $s = \sqrt{1-c^2} = \sin\theta$

$m \backslash \ell$	0	1	2	3
3				$-15s^3$
2			$3s^2$	$15cs^2$
1		$-s$	$-3cs$	$-\frac{3}{2}(5c^2-1)s$
0	1	c	$\frac{1}{2}(3c^2-1)$	$\frac{1}{2}(5c^3-3c)$
−1		$\frac{1}{2}s$	$\frac{1}{2}cs$	$\frac{1}{8}(5c^2-1)s$
−2			$\frac{1}{8}s^2$	$\frac{1}{8}cs^2$
−3				$\frac{1}{48}s^3$