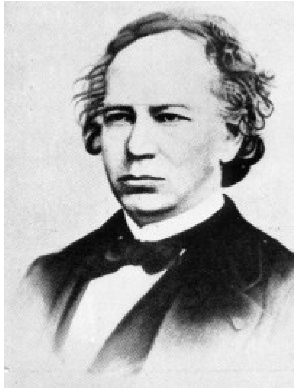
4. Hermite and Laguerre polynomials

4.1 Hermite polynomials from a generating function

We will see that Hermite polynomials are solutions to the radial part of the Schrodinger Equation for the simple harmonic oscillator.

Learning outcome: Derive Hermite's equation and the Hermite recurrence relations from the generating function.

Just like Legendre polynomials and Bessel functions, we may define Hermite polynomials $H_n(x)$ via a generating function.



Charles Hermite
1822-1901

$$g(x,t) = e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$$

We could, of course, use this to derive the individual polynomials, but this is very tedious. It is better to derive recurrence relations.

$$g(x,t) = e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$$

Differentiate with respect to t:

$$\frac{\partial}{\partial t}g(x,t) = (-2t+2x)\,e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x)n\frac{t^{n-1}}{n!}$$

Expand the terms, and put the generating function in again:

$$-2\sum_{n=0}^{\infty} H_n(x)\frac{t^{n+1}}{n!} + 2x\sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!} = \sum_{n=1}^{\infty} H_n(x)\frac{t^{n-1}}{(n-1)!}$$

Relabel:

$$-2\sum_{n=1}^{\infty} nH_{n-1}(x)\frac{t^n}{n!} + 2x\sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!} = \sum_{n=0}^{\infty} H_{n+1}(x)\frac{t^n}{n!}$$

Equating coefficients of t^n:

$$\Rightarrow \quad \boxed{H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)} \qquad (n \geq 1)$$

$$g(x,t) = e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$$

Differentiate with respect to x:

$$\frac{\partial}{\partial x} g(x,t) = 2t\,e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n'(x)\frac{t^n}{n!}$$

Stick in g:

$$2\sum_{n=0}^{\infty} H_n(x)\frac{t^{n+1}}{n!} = \sum_{n=1}^{\infty} H_n'(x)\frac{t^n}{n!}$$

Relabel:

$$2\sum_{n=1}^{\infty} H_{n-1}(x)\frac{t^n}{(n-1)!} = \sum_{n=1}^{\infty} H_n'(x)\frac{t^n}{n!}$$

Equating coefficients of t^n:

$$\Rightarrow \quad \boxed{H_n'(x) = 2nH_{n-1}(x)} \qquad (n \geq 1)$$

We can use these recurrence relations to derive the Hermite differential equation (much easier than Legendre's!).

$$\left.\begin{aligned} H_{n+1}(x) &= 2xH_n(x) - 2nH_{n-1}(x) \\ H_n'(x) &= 2nH_{n-1}(x) \end{aligned}\right\} \quad \Rightarrow \quad H_{n+1}(x) = 2xH_n(x) - H_n'(x)$$

Differentiate with respect to x:

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

$$2(n+1)H_n(x) = 2H_n(x) + 2xH_n'(x) - H_n''(x)$$

$$\Rightarrow \quad \boxed{H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0}$$

This is **Hermite's equation**.

Learning outcome: Use a generating function and recurrence relations to find the first few Hermite polynomials.

Generating function: $$\sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!} \;=\; e^{-t^2+2tx}$$

$$\Rightarrow H_0(x) + H_1(x)t + \mathcal{O}(t^2) \;=\; 1 - t^2 + 2tx + \mathcal{O}(t^2) \quad \Rightarrow \begin{cases} t^0: & \rightarrow H_0(x) = 1 \\ t^1: & \rightarrow H_1(x) = 2x \end{cases}$$

Now use the recurrence relation,

$$H_{n+1}(x) \;=\; 2xH_n(x) \;-\; 2nH_{n-1}(x)$$

$$H_2(x) \;= 2xH_1(x) - 1 \times 2H_0(x) \;= 4x^2 - 2$$

$$H_3(x) \;= 2xH_2(x) - 2 \times 2H_1(x) \;= 8x^3 - 4x - 8x = 8x^3 - 12x$$

$$H_4(x) \;= 2xH_3(x) - 3 \times 2H_2(x) \;= 16x^4 - 24x^2 - (24x^2 - 12) = 16x^4 - 48x^2 + 12$$

4.2 Properties of Hermite polynomials

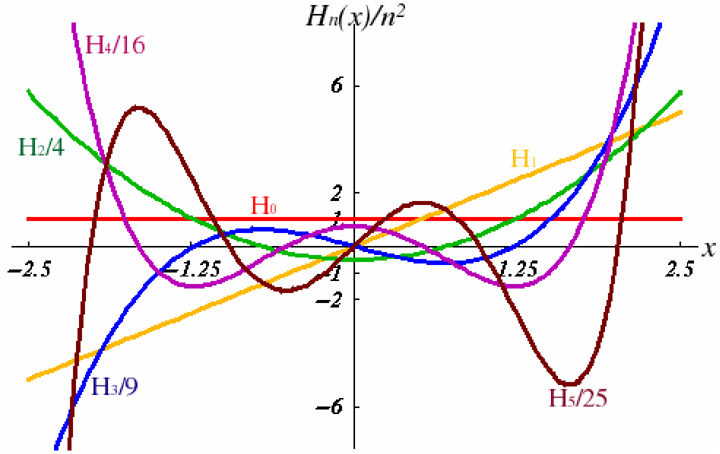
Symmetry about x=0:

$$g(-x,-t) = e^{-(-t)^2+2(-t)(-x)} = e^{-t^2+2tx} = g(x,t)$$

$$\Rightarrow \quad \sum_{n=0}^{\infty} H_n(-x)\frac{(-t)^n}{n!} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$$

$$\Rightarrow \quad H_n(-x) = (-1)^n H_n(x)$$

(just like for Legendre polynomials)



There also exists a specific series form:

$$H_n(x) = \sum_{m=0}^{n/2} (-1)^m (2x)^{n-2m} \frac{n!}{(n-2m)!m!}$$

Exercise: Use this series to verify the first few Hermite polynomials.

Exercise:

Writing $g(x,t) = e^{x^2} e^{-(t-x)^2}$ show that

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right)$$

This is Rodrigues' equation for Hermite polynomials.

(Hint: work out $\left.\frac{\partial^n g}{\partial t^n}\right|_{t=0}$ and observe that $\frac{\partial}{\partial t} e^{-(t-x)^2} = -\frac{\partial}{\partial x} e^{-(t-x)^2}$)

Learning outcome: Write down the Hermite polynomial orthogonality condition.

Starting from Hermite's equation: $H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0$

$$\Rightarrow \quad \frac{d}{dx}\left(e^{-x^2}\frac{d}{dx}H_n(x)\right) + 2n\,e^{-x^2}\,H_n(x) = 0$$

we proceed much the same way as we did for Legendre polynomials.

$$\Rightarrow \quad H_m(x)\,\frac{d}{dx}\left[e^{-x^2}\,\frac{d}{dx}\,H_n(x)\right] - H_n(x)\,\frac{d}{dx}\left[e^{-x^2}\,\frac{d}{dx}\,H_m(x)\right]$$

$$= -H_m(x)\,2n\,e^{-x^2}\,H_n(x) + H_n(x)\,2m\,e^{-x^2}\,H_m(x)$$

Integrate this over x from $-\infty$ to ∞, integrating the left-hand-side by parts.

$$\int_{-\infty}^{\infty} H_m(x)\,\frac{d}{dx}\left[e^{-x^2}\,\frac{d}{dx}\,H_n(x)\right]\,dx = \left[H_m(x)\,e^{-x^2}\,\frac{d}{dx}\,H_n(x)\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\left[\frac{d}{dx}\,H_m(x)\right]\,e^{-x^2}\,\frac{d}{dx}\,H_n(x)\,dx$$

zero — symmetric in $n \leftrightarrow m$

$$\Rightarrow \quad 2(m-n)\int_{-\infty}^{\infty} H_n(x)H_m(x)\,e^{-x^2}\,dx = 0$$

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

We say that Hermite polynomials are orthogonal on the interval [-∞,∞] with a weighting e^{-x^2}

$$\int_{-\infty}^{\infty} g^2(x,t) e^{-x^2}\, dx = \int_{-\infty}^{\infty} e^{-2t^2+4tx-x^2}\, dx = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{t^{n+m}}{n!m!} \int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2}\, dx$$

$$\int_{-\infty}^{\infty} e^{-(x-2t)^2} e^{2t^2}\, dx \qquad\qquad \sum_{n=0}^{\infty} \frac{t^{2n}}{(n!)^2} \int_{-\infty}^{\infty} [H_n(x)]^2\, e^{-x^2}\, dx$$

$$= e^{2t^2} \int_{-\infty}^{\infty} e^{-x^2}\, dx = e^{2t^2}\sqrt{\pi}$$

$$= \sqrt{\pi} \sum_{n=0}^{\infty} \frac{2^n}{n!} t^{2n}$$

$$\left(\begin{aligned} \left[\int_{-\infty}^{\infty} e^{-x^2}\, dx\right]^2 &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\, e^{-x^2-y^2} \\ &= \int_0^{2\pi} d\theta \int_0^{\infty} dr\, r\, e^{-r^2} = 2\pi \left[-\frac{1}{2} e^{-r^2}\right]_0^{\infty} = \pi \end{aligned}\right)$$

Equating powers of t^{2n} gives $\int_{-\infty}^{\infty} [H_n(x)]^2\, e^{-x^2}\, dx = 2^n \sqrt{\pi}\, n!$

$$\Rightarrow \quad \boxed{\int_{-\infty}^{\infty} H_n(x) H_m(x)\, e^{-x^2}\, dx = 2^n \sqrt{\pi}\, n!\, \delta_{nm}}$$

Exercise: For a continuous function, I can write $f(x) = \sum_{n=0}^{\infty} c_n H_n(x)$. Show that

$$c_n = \frac{1}{2^n \sqrt{\pi} n!} \int_{-\infty}^{\infty} f(x)\, H_n(x) e^{-x^2}\, dx$$

Sometimes people remove the weighting by redefining the function: $\varphi_n(x) \equiv e^{-x^2/2} H_n(x)$

$$\Rightarrow \qquad \int_{-\infty}^{\infty} \varphi_n(x)\varphi_m(x)\, dx = 2^n \sqrt{\pi} n!\, \delta_{nm}$$

Now this looks like a “traditional” orthogonality relation.

$$H_n(x) = e^{x^2/2}\varphi_n(x) \qquad \Rightarrow \qquad H_n'(x) = x\, e^{x^2/2}\, \varphi_n(x) + e^{x^2/2}\varphi_n'(x)$$

$$\Rightarrow \qquad H_n''(x) = e^{x^2/2}\varphi_n''(x) + 2x\, e^{x^2/2}\, \varphi_n'(x) + (1+x^2)\, \varphi_n(x)$$

Then Hermite’s equation $H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0$ becomes

$$\boxed{\varphi_n''(x) + (1 - x^2 + 2n)\, \varphi_n(x) = 0}$$

4.3 Hermite polynomials and the Quantum Harmonic Oscillator

Learning Outcome: Solve the quantum harmonic oscillator in terms of Hermite polynomials.

Recall our earlier discussion of the time-independent Schrödinger equation. That was in 3-dimensions, but here I will simplify to one dimension again,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\,\psi(x),$$

where m is the particle mass, and E is its energy.

For the simple harmonic oscillator, $V(x) = \frac{1}{2}m\omega^2 x^2$, so the equation becomes

$$\psi''(x) + \left(-\frac{m^2\omega^2}{\hbar^2}x^2 + \frac{2mE}{\hbar^2}\right)\psi(x) = 0$$

Notice that this looks awfully like the equation we just had on the previous slide:

$$\varphi_n''(x) + (1 - x^2 + 2n)\,\varphi_n(x) = 0$$

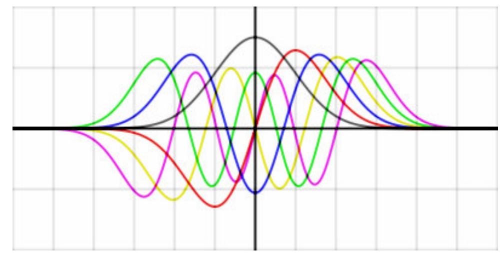
Our reweighted Hermite polynomials are solutions of the Quantum Harmonic Oscillator!

Let's write $y = ax$ with $a = \sqrt{\frac{m\omega}{\hbar}}$ so we get

$$\frac{d^2}{dy^2}\psi\left(y/a\right) + \left(-y^2 + \frac{2mE}{\hbar^2 a^2}\right)\psi\left(y/a\right) = 0$$

Comparing the two equations, we see that we have solutions,

$$\psi_n(x) = \sqrt{\frac{a}{2^n\sqrt{\pi}n!}}\, e^{-a^2x^2/2} H_n\left(ax\right)$$



where the normalization constant in front ensures that $\int_{-\infty}^{\infty} \left|\psi_n(x)\right|^2\, dx = 1$, and,

the energy is given by the equation

$$\frac{2mE}{\hbar^2 a^2} = 1 + 2n \quad \Rightarrow \quad \frac{2E}{\hbar\omega} = 1 + 2n \quad \Rightarrow \quad E = \hbar\omega\left(n + \frac{1}{2}\right)$$

Have you seen this somewhere before?

You probably solved this elsewhere using ladder operators. This works (in part) because of the Hermite recurrence relation $H_n'(x) = 2nH_{n-1}(x)$.

Writing $\varphi_n(x) = \sqrt{\frac{1}{2^n\sqrt{\pi}n!}}\, e^{-x^2/2} H_n(x)$ for simplicity (ie. set a=1 for now)

Then $\frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right)\varphi_n(x) = \sqrt{\frac{1}{2^{n+1}\sqrt{\pi}n!}}\left(x + \frac{d}{dx}\right) e^{-x^2/2} H_n(x)$

$$= \sqrt{\frac{1}{2^{n+1}\sqrt{\pi}n!}}\left(x\, e^{-x^2/2}\, H_n(x) - x\, e^{-x^2/2}\, H_n(x) + e^{-x^2/2}\, H_n'(x)\right)$$

$$= \sqrt{\frac{1}{2^{n+1}\sqrt{\pi}n!}}\left(e^{-x^2/2}\, 2n\, H_{n-1}(x)\right) = \sqrt{\frac{n}{2^{n-1}\sqrt{\pi}(n-1)!}}\left(e^{-x^2/2}\, H_{n-1}(x)\right)$$

$$= \sqrt{n}\,\varphi_{n-1}(x)$$

This is a **lowering operator**.

➡ **Exercise**: Use recurrence relations to show that the operator $\frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)$ is a raising operator. Can you show it using the Rodrigues' equation?

But why is the quantum harmonic oscillator quantized?

We have seen why $E = \hbar\omega\,(n + \frac{1}{2})$, and how to move from one energy state to another using ladder operators, but we still have no reason for why n must be an integer!

Indeed, Hermite's equation $H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0$ **does** have solutions for non-integer values of n.

Plugging $H_n(x) = \sum_{k=0}^{\infty} c_k x^k$ into the equation, one finds a solution

$$H_n(x) = c_0 \left[1 + \frac{2(-n)}{2!}x^2 + \frac{2^2(-n)(2-n)}{4!}x^4 + \ldots\right] + c_1 \left[x + \frac{2(1-n)}{3!}x^3 + \frac{2^2(1-n)(3-n)}{5!}x^5 + \ldots\right]$$

which is valid for non-integer n. (This is known as a Hermite "function".)

For integer n, this solution (or to be more precise, half of it) will truncate to give Hermite polynomials.

For non-integer n, it does not truncate and one can show that the terms grow like $x^n e^{x^2/2}$
These solutions do not satisfy the boundary condition $\psi(x) \to 0$ as $x \to \infty$, so must be discarded and the harmonic oscillator is quantized.

4.4 Laguerre polynomials and the hydrogen atom

Learning outcome: Understand the importance of Laguerre polynomials to the solution of Schrodinger's equation for the hydrogen atom.

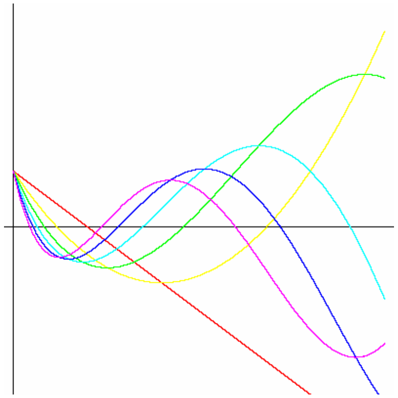
Edmond Laguerre
1834-1886

Generating function:

$$g(x,t) = \frac{e^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} L_n(x) t^n$$

Exercise: Starting from the generating function, prove the two recurrence relations

$$(n+1)L_{n+1}(x) = (2n+1-x)L_n(x) - nL_{n-1}(x)$$
$$xL_n'(x) = nL_n(x) - nL_{n-1}(x)$$



Also, show $L_n(0) = 1$ and find expressions for the first 4 polynomials.

Following a similar method to that used for Legendre and Hermite polynomials, we can show that the Laguerre polynomials are orthogonal over the interval [0,∞] with a weighting e^{-x}, i.e.

$$\int_0^\infty L_n(x)L_m(x)e^{-x}dx = \delta_{nm}$$

They satisfy the **Laguerre equation**:

$$xL_n''(x) + (1-x)L_n'(x) + nL_n(x) = 0$$

and have a Rodrigues' formula

$$L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}\left(x^n e^{-x}\right)$$

(These results can be proven using similar methods to those used earlier for Legendre and Hermite polynomials. If you are feeling assiduous feel free to do these as an exercise.)

Associated Laguerre polynomials are obtained by differentiating “regular” Laguerre polynomials (just as for Legendre).

$$L_n^k(x) = (-1)^n \frac{d^k}{dx^k} L_{n+k}(x)$$

Exercise: Show that $L_n^k(x)$ are solutions to the **associated Laguerre equation**

$$x L_n^{k\,\prime\prime}(x) + (k+1-x) L_n^{k\,\prime}(x) + n L_n^k(x) = 0$$

These are also orthogonal with $\int_0^\infty L_n^k(x) L_m^k(x) x^k e^{-x} dx = \frac{(n+k)!}{n!} \delta_{nm}$

Recall our investigation of the Schrödinger equation in spherical coordinates with $V = V(r)$.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\underline{r}) + V\psi(\underline{r}) = E\psi(\underline{r})$$

Separating $\psi(\underline{r}) = R(r)Y_l^m(\theta,\phi)$ resulted in spherical harmonics

$$Y_l^m(\theta,\phi) = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\,e^{im\phi}\,P_l^m(\cos\theta)$$

and a radial equation $\frac{d}{dr}\left[r^2\frac{dR(r)}{dr}\right] - \frac{2m}{\hbar^2}(V(r)-E)\,r^2\,R(r) - l(l+1)R(r) = 0$

For the hydrogen atom (that is, with $\psi(\underline{r})$ the wavefunction for an electron orbiting a proton), the potential is the Coulomb potential,

$$V(\underline{r}) = \frac{-e^2}{4\pi\epsilon_0 r}$$

To make the maths a wee bit cleaner, let's make the following redefinitions:

$$\rho = \alpha r\,, \qquad \alpha = \sqrt{-\frac{8mE}{\hbar^2}}, \qquad \lambda = \frac{me^2}{2\pi\epsilon_0 \alpha \hbar^2}\,, \qquad \chi(\rho) = R(r), \text{ with } E < 0$$

(we regard E=0 at ∞)

Then

$$\frac{d}{dr}\left[r^2 \frac{dR(r)}{dr}\right] - \frac{2m}{\hbar^2}\left(\frac{-e^2}{4\pi\epsilon_0 r} - E\right) r^2 R(r) - l(l+1)R(r) = 0$$

becomes

$$\frac{d}{d\rho}\left[\rho^2 \frac{d\chi(\rho)}{d\rho}\right] + \left(\lambda\rho - \frac{1}{4}\rho^2 - l(l+1)\right)\chi(\rho) = 0$$

which has solutions containing associated Laguerre polynomials,

$$\chi(\rho) = e^{-\rho/2}\,\rho^l\, L^{2l+1}_{\lambda-l-1}(\rho)$$

Exercise: Plug the above result into the radial equation to recover the associated Laguerre equation for $L(\rho)$.

Just as for the Hermite equation, solutions exist for non-integer λ-l-1 but these diverge as r$\rightarrow\infty$ and must be discarded. The boundary conditions quantize the energy of the Hydrogen atom.

Fixing λ to be an integer n,

$$E_n = -\frac{\alpha^2\hbar^2}{8m} = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{2a_0}\frac{1}{n^2}$$

where $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} = \frac{2}{n\alpha}$ is the **Bohr radius**.

Also, hydrogen wavefunctions are,

$$\psi_{nlm}(r,\theta,\phi) = N_{nlm}\, e^{-\alpha r/2}\,(\alpha r)^l\, L^{2l+1}_{n-l-1}\,(\alpha r)\, Y_l^m(\theta,\phi)$$

where N_{nlm} is a normalization coefficient.

To find the normalization coefficient we need

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} |\psi_{nlm}(r,\theta,\phi)|^2\, r^2 \sin\theta\, dr d\theta d\phi \;=\; \alpha^{-3}\int_0^{\infty} [\chi(\rho)]^2\, \rho^2 d\rho$$

$$= N_{nlm}^2 \frac{1}{\alpha^3}\int_0^{\infty} e^{-\rho}\,\rho^{2l+2}\, L_{n-l-1}^{2l+1}(\rho) L_{n-l-1}^{2l+1}(\rho)\, d\rho \;=\; N_{nlm}^2 \frac{2n}{\alpha^3}\frac{(n+l)!}{(n-l-1)!} \;=\; 1$$

Notice the $2n$ here. This is because we don't quite have the orthogonality condition for the associated Laguerre polynomials we had before - we have an extra power of ρ. This result is most easily proven with a recurrence relation,

$$xL_n^k = (2n{+}k{+}1)L_m^k - (n{+}k)L_{n-1}^k - (n{+}1)L_{n+1}^k$$

Finally, the electron wavefunction in the hydrogen atom is

$$\psi_{nlm}(r,\theta,\phi) \;=\; \left[\frac{\alpha^3}{2n}\frac{(n-l-1)!}{(n+l)!}\right]^{1/2} (\alpha r)^l\, e^{-\alpha r/2} L_{n-l-1}^{2l+1}(\alpha r)\, Y_l^m(\theta,\phi)$$