Legendre Polynomials

Bernd Schröder

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3. The solutions of both equations *must* be finite on $[-1,1]$.
4. Because 0 is an ordinary point of the equation, it is natural to attempt a series solution.

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$$\begin{aligned} & \left(2c_2+\lambda c_0\right)+\left(6c_3x-2c_1x+\lambda c_1x\right)+ \\ \sum_{k=2}^{\infty}\left[(k+2)(k+1)c_{k+2}-k(k-1)c_k-2kc_k+\lambda c_k\right]x^k & = 0 \end{aligned}$$

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Matching coefficients leads to $c_2=-\frac{\lambda}{2}c_0$, $c_3=-\frac{\lambda-2}{6}c_1$, and for $k\geq 2$

$$
c_{k+2} \quad = \quad \frac{k(k-1)+2k-\lambda}{(k+2)(k+1)}c_k=\frac{k(k+1)-\lambda}{(k+2)(k+1)}c_k.
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3. Therefore, these solutions are not physically feasible, because the polar part $y\big(\cos(\phi)\big)$ of the solution of $\Delta u=f(\rho)u$ should not go to infinity as we approach the z-axis. (For QM, the explanation involves integrability issues.)

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7. But the entries $c_{l+(2k+1)}$ may still not be zero.
8. By choosing one of c_0 (or c_1) equal to zero, we can make all even-numbered coefficients (or all odd-numbered coefficients) equal to zero.
9. So the solutions we are interested in will be polynomials with even powers (for $\lambda=l(l+1)$ and l even) or polynomials with odd powers (for $\lambda=l(l+1)$ and l odd).

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&= \frac{k(k+1)-l(l+1)}{(k+2)(k+1)}c_k \\
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\end{aligned}
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&= \frac{k^2+k-l^2-l}{(k+2)(k+1)}c_k \\
&= \frac{(k+l)(k-l)+(k-l)}{(k+2)(k+1)}c_k
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&= \frac{(k+l)(k-l)+(k-l)}{(k+2)(k+1)}c_k \\
&= \frac{(k+l+1)(k-l)}{(k+2)(k+1)}c_k
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c_{k+2} &= \frac{k(k+1)-\lambda}{(k+2)(k+1)}c_k \\
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&= \frac{k^2+k-l^2-l}{(k+2)(k+1)}c_k \\
&= \frac{(k+l)(k-l)+(k-l)}{(k+2)(k+1)}c_k \\
&= \frac{(k+l+1)(k-l)}{(k+2)(k+1)}c_k \\
&= -\frac{(l-k)(l+k+1)}{(k+2)(k+1)}c_k
\end{aligned}$$

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&\vdots \\
c_{2n} &= (-1)^n\frac{l(l-2)\cdots\big(l-2(n-1)\big)\cdot(l+2n-1)(l+2n-3)\cdots(l+1)}{(2n)!}c_0
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&= (-1)^n \frac{(l+2n-1)(l+2n-3)\cdots(l+1)}{(2n)!}\,\frac{l(l-2)\cdots\big(l-2(n-1)\big)}{l(l-2)\cdots\big(l-2(n-1)\big)}\,\frac{2^{\frac{l}{2}}\left(\frac{l}{2}\right)!}{2^{\frac{l}{2}-n}\left(\frac{l}{2}-n\right)!}c_0 \\
&= (-1)^n \frac{(l+2n-1)(l+2n-3)\cdots(l+1)}{(2n)!}\,\frac{l!2^{\frac{l}{2}+n}\left(\frac{l}{2}+n\right)!}{l!2^{\frac{l}{2}+n}\left(\frac{l}{2}+n\right)!}\,\frac{2^{\frac{l}{2}}\left(\frac{l}{2}\right)!}{2^{\frac{l}{2}-n}\left(\frac{l}{2}-n\right)!}c_0
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&= (-1)^n \frac{(l+2n-1)(l+2n-3)\cdots(l+1)}{(2n)!}\frac{l(l-2)\cdots\big(l-2(n-1)\big)}{l(l-2)\cdots\big(l-2(n-1)\big)}\frac{2^{\frac{l}{2}}\left(\frac{l}{2}\right)!}{2^{\frac{l}{2}-n}\left(\frac{l}{2}-n\right)!}c_0 \\
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&= (-1)^n \frac{(l+2n)!}{(2n)!l!}\frac{\left[\left(\frac{l}{2}\right)!\right]^2}{\left(\frac{l}{2}+n\right)!\left(\frac{l}{2}-n\right)!}c_0
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&= (-1)^k \frac{(2l-2k)!}{2^l(l-2k)!(l-k)!k!} (-1)^{\frac{l}{2}} \frac{2^l\left[\left(\frac{l}{2}\right)!\right]^2}{l!} c_0
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Choosing $c_0 = (-1)^{\frac{l}{2}} \dfrac{l!}{2^l \left[\left(\frac{l}{2}\right)!\right]^2}$ gives

$$P_l(x) = \sum_{k=0}^{\left\lfloor \frac{l}{2} \right\rfloor} (-1)^k \frac{(2l-2k)!}{2^l k!(l-k)!(l-2k)!} x^{l-2k},$$

which is the customary way the Legendre polynomials are stated.

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(The generalized Legendre equation is good reading.)

Electron Orbitals

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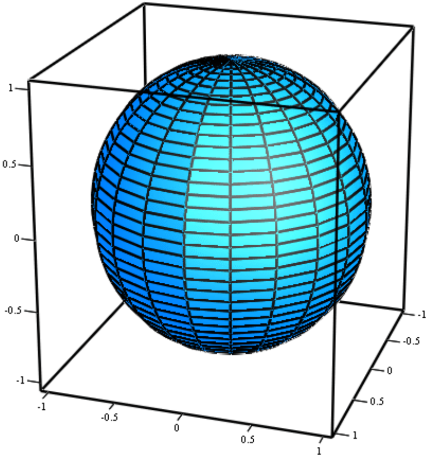
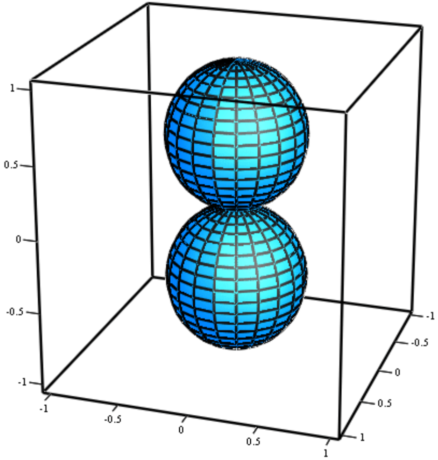
5. So $\rho = P_n\big(\cos(\phi)\big)$ should give the "shapes" of the orbitals when P_n is a Legendre polynomial.
6. "Shape" must be carefully interpreted. Large values for $\rho(\phi) = P_n(\phi)$ in the picture indicate a large probability (density) that the electron's location's polar angle is around the angle ϕ.

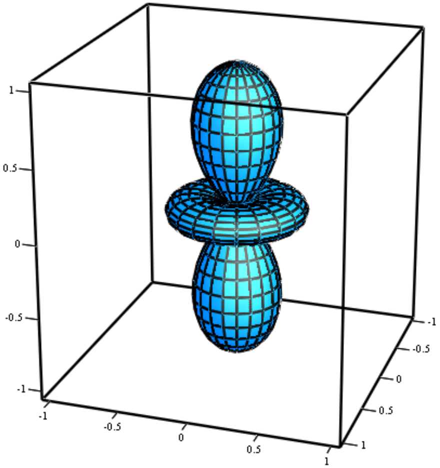
$\rho = \left|P_0(\cos(\phi))\right|$: 1s Orbital



$\rho = |P_1(\cos(\phi))|$: 2p Orbital



$\rho = |P_2(\cos(\phi))|$: 3d Orbital



$\rho = \left|P_3(\cos(\phi))\right|$: 4f Orbital