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# Legendre Polynomials, Dipole Moments, Generating Functions etc..

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## I. SYNOPSIS

A standard treatment of aspects of Legendre Polynomials is treated here. In addition, the dipole moment expansion in Legendre Polynomials is introduced. Finally, the inter-electronic repulsive energy between electrons is expanded in a Legendre Polynomial like series.

## II. A GENERATING FUNCTION FOR LEGENDRE POLYNOMIALS

The technically correct generating function for Legendre polynomials is obtained using the equation

$$\frac{1}{\sqrt{1-2xu+u^2}} = \sum_0^\infty P_n(x)u^n \tag{2.1}$$

We expand the denominator using the binomial theorem,

$$\frac{1}{(1+y)^m} = 1 - my + \frac{m(m+1)}{2!}y^2 - \frac{m(m+1)(m+2)}{3!}y^3 + \cdots$$

where $m = \frac{1}{2}$ and the series converges when $y < 1$. Notice that it is an alternating series. Identifying $y = u^2 - 2xu$ we have

$$\frac{1}{(1-2xu+u^2)^{\frac{1}{2}}} = 1 - (\frac{1}{2})(u^2-2xu) + \frac{(\frac{1}{2})((\frac{1}{2})+1)}{2!}(u^2-2xu)^2 - \frac{(\frac{1}{2})((\frac{1}{2})+1)((\frac{1}{2})+2)}{3!}(u^2-2xu)^3 + \cdots$$

which we now re-arrange in powers of u (in the mode required by Equation 2.1), obtaining

$$\frac{1}{(1-2xu+u^2)^{\frac{1}{2}}} = 1 - \frac{u^2}{2} + xu + \frac{(\frac{3}{4})}{2!}(u^4 - 4xu^3 + 4x^2u^2) - \frac{(\frac{1}{2})(\frac{3}{2})(\frac{5}{2})}{3!}(u^2-2xu)^3 + \cdots$$

which is, rearranging

$$\frac{1}{(1-2xu+u^2)^{\frac{1}{2}}} = 1 + xu - \frac{u^2}{2} + \frac{(\frac{3}{4})}{2!}4x^2u^2 - \frac{(\frac{3}{4})}{2!}4xu^3 + \frac{(\frac{3}{4})}{2!}u^4 - \frac{(\frac{1}{2})(\frac{3}{2})(\frac{5}{2})}{3!}\left(u^6 - 6xu^5 + 12x^2u^4 - 16x^3u^3\right) + \cdots$$

or, collecting terms in powers of u, we have

$$\frac{1}{(1-2xu+u^2)^{\frac{1}{2}}} = \tag{2.2}$$

$$1 + xu + \frac{1}{2}\left(3x^2-1\right)u^2 + \left(-\frac{(\frac{3}{4})}{2!}4x + \frac{(\frac{1}{2})(\frac{3}{2})(\frac{5}{2})}{3!}16x^3\right)u^3 + \left(\frac{(\frac{3}{4})}{2!} - \frac{(\frac{1}{2})(\frac{3}{2})(\frac{5}{2})}{3!}12x^2\right)u^4 - \frac{(\frac{1}{2})(\frac{3}{2})(\frac{5}{2})}{3!}(-6xu^5) - \frac{(\frac{1}{2})(\frac{3}{2})(\frac{5}{2})}{3!}u^6 + \cdots \tag{2.3}$$

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where the quadratic terms (in u, i.e. $3x^2 - 1$) is the familiar spherical harmonic associated with the $d_{z^2}$ orbital, among other things.

## III. AN ALTERNATIVE GENERATING FUNCTION METHOD

Another method of introducing Legendre Polynomials is through the inter electronic potential energy function in Helium atom's Hamiltonian. Since this method is very important in Quantum Mechanical computations concerning poly-electronic atoms and molecules, it is worth our attention. When one considers the Hamiltonian of the Helium Atom's electrons (for example), one has

$$-\frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{r_{12}} \tag{3.1}$$

where $r_{12}$ is the distance between electron 1 and electron 2, i.e., it is the electron-electron repulsion term. We examine this term in this discussion. We can write this electron-electron repulsion term as

$$\frac{1}{r_{12}} = \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\vartheta}} \tag{3.2}$$

where $r_1$ and $r_2$ are the distances from the nucleus to electrons 1 and 2 respectively. $\vartheta$ is the angle *between the vectors from the nucleus to electron 1 and electron 2*. It is required that we do this is two domains, one in which $r_1 > r_2$ and one in which $r_2 > r_1$. This is done for convergence reasons.

For the former case, we define

$$\zeta = \frac{r_2}{r_1}$$

so that $\zeta < 1$, and Equation 3.2 becomes

$$\frac{1}{r_{12}} = \frac{1}{r_1}\frac{1}{\sqrt{1+\zeta^2 - 2\zeta\cos\vartheta}} \tag{3.3}$$

which we now expand in a power series in $\cos\vartheta$ (which will converge while $\zeta < 1$). We have

$$\frac{1}{r_1}\frac{1}{\sqrt{1+\zeta^2 - 2\zeta\cos\vartheta}} = \tag{3.4}$$

$$\frac{1}{r_1}\left(1 + \frac{1}{1!}\left.\frac{d\left(\frac{1}{\sqrt{1+\zeta^2-2\zeta\cos\vartheta}}\right)}{d\cos\vartheta}\right|_{\cos\vartheta=0}\cos\vartheta + \frac{1}{2!}\left.\frac{d^2\left(\frac{1}{\sqrt{1+\zeta^2-2\zeta\cos\vartheta}}\right)}{d\cos\vartheta^2}\right|_{\cos\vartheta=0}\cos^2\vartheta + \cdots\right) \tag{3.5}$$

It is customary to change notation from $\cos\vartheta$ to $\mu$, so

$$\frac{1}{r_{12}} = \frac{1}{r_1}\frac{1}{\sqrt{1+\zeta^2 - 2\zeta\mu}} \tag{3.6}$$

which we now expand in a power series in $\mu$ (which will converge while $\zeta < 1$). We have

$$\frac{1}{r_1}\frac{1}{\sqrt{1+\zeta^2 - 2\zeta\mu}} = \frac{1}{r_1}\left(1 + \frac{1}{1!}\left.\frac{d\left(\frac{1}{\sqrt{1+\zeta^2-2\zeta\mu}}\right)}{d\mu}\right|_{\mu=1}\mu + \frac{1}{2!}\left.\frac{d^2\left(\frac{1}{\sqrt{1+\zeta^2-2\zeta\mu}}\right)}{d\mu^2}\right|_{\mu=1}\mu^2 + \cdots\right) \tag{3.7}$$

$$\frac{1}{r_1}\frac{1}{\sqrt{1+\zeta^2 - 2\zeta\mu}} =$$

$$\frac{1}{r_1}\left(1 + \frac{1}{1!}\left.\frac{-1}{2}(1+\zeta^2-2\zeta\mu)^{-\frac{3}{2}}(-2\zeta)\right|_{\mu=1}\mu + \frac{1}{2!}\left.\frac{d^2\left(\frac{1}{\sqrt{1+\zeta^2-2\zeta\mu}}\right)}{d\mu^2}\right|_{\mu=1}\mu^2 + \cdots\right) \tag{3.8}$$

which is

$$\frac{1}{r_1}\frac{1}{\sqrt{1+\zeta^2-2\zeta\mu}} = \frac{1}{r_1}\left(1-\frac{1}{2}(1+\zeta^2-2\zeta)^{-\frac{3}{2}}\,(-2\zeta)\,\mu + \frac{1}{2!}\,\frac{d\left(\frac{-1}{2}(1+\zeta^2-2\zeta\mu)^{-\frac{3}{2}}\,(-2\zeta)\right.}{d\mu}\bigg|_{\mu=1}\mu^2+\cdots\right) \tag{3.9}$$

i.e.,

$$\frac{1}{r_1}\frac{1}{\sqrt{1+\zeta^2-2\zeta\mu}} = \frac{1}{r_1}\left(1-\frac{1}{2}(1+\zeta^2-2\zeta)^{-\frac{3}{2}}\,(-2\zeta)\,\mu + \frac{1}{2!}\,\frac{d\left((1+\zeta^2-2\zeta\mu)^{-\frac{3}{2}}\,(\zeta)\right)}{d\mu}\bigg|_{\mu=1}\mu^2+\cdots\right) \tag{3.10}$$

which is, after the second differentiation

$$\frac{1}{r_1}\frac{1}{\sqrt{1+\zeta^2-2\zeta\mu}} = \frac{1}{r_1}\left(1-\frac{1}{2}(1+\zeta^2-2\zeta)^{-\frac{3}{2}}\,(-2\zeta)\,\mu + \frac{1}{2!}\left(-\frac{3}{2}(1+\zeta^2-2\zeta\mu)^{-\frac{5}{2}}(-2\zeta)\zeta\right)\bigg|_{\mu=1}\mu^2+\cdots \tag{3.11}$$

Cleaning up, a bit, we have

$$\frac{1}{r_{12}} = \frac{1}{r_1}\left(1+\left((1+\zeta^2-2\zeta)^{-\frac{3}{2}}\zeta\right)\mu + \frac{1}{2!}\left(+2\frac{3}{2}(1+\zeta^2-2\zeta)^{-\frac{5}{2}}\zeta^2\right)\mu^2+\cdots\right) \tag{3.12}$$

where we look forward to Equation 4.1, to see similarities. Remember that we've only handled the case with $\zeta = r_1 > r_2$.

## IV. THE EXPANSION OF A FINITE DIPOLE IN LEGENDRE POLYNOMIALS

There is yet another way to see Legendre Polynomials in action, through the expansion of the potential energy of point dipoles. To start, we assume that we have a dipole at the origin, with its positive charge (q) at (0,0,-a/2) and its negative charge (-q) at (0,0,+a/2), so that the "bond length" is "a", and therefore the "dipole moment" is "q a".

At some point P(x,y,z), located (also) at r,$\vartheta$,$\phi$, we have that the potential energy due to these two point charges is

$$U(x,y,z,a) = \frac{-q}{\sqrt{x^2+y^2+(z-a/2)^2}} + \frac{q}{\sqrt{x^2+y^2+(z+a/2)^2}}$$

which is just Coulomb's law.

If we expand this potential energy as a function of "a", the "bond distance", we have

$$U(x,y,z,a) = U(x,y,z,0) + \frac{1}{1!}\,\frac{dU}{da}\bigg|_{a=0} a + \frac{1}{2!}\,\frac{d^2U}{da^2}\bigg|_{a=0} a^2 + \frac{1}{3!}\,\frac{d^3U}{da^3}\bigg|_{a=0} a^3 + \cdots$$

All we need do, now, is evaluate these derivatives. We have, for the first

$$\frac{1}{1!}\,\frac{dU}{da}\bigg|_{a=0} = q\left(-\left[-\left(\frac{1}{2}\right)\frac{2(z-a/2)(-\frac{1}{2})}{(x^2+y^2+(z-a/2)^2))^{\frac{3}{2}}}\right] + \left[-\left(\frac{1}{2}\right)\frac{2(z+a/2)(\frac{1}{2})}{(x^2+y^2+(z+a/2)^2))^{\frac{3}{2}}}\right]\right)$$

which is, in the limit $a \to 0$,

$$q\left(-\frac{z}{r^3}\right)$$

so, we have, so far,

$$U(x,y,z,a) = 0 - qa\left(\frac{z}{r^3}\right) + \cdots = -qa\left(\frac{\cos\vartheta}{r^2}\right) + \cdots \tag{4.1}$$

i.e., to the dipolar form.

For the second derivative, we take the derivative of the first derivative:

$$\frac{1}{2!}\left.\frac{d\frac{dU}{da}}{da}\right|_{a=0} = -q\frac{1}{2\times 2!}\left(\frac{d\left(\left[\frac{(z-a/2)}{(x^2+y^2+(z-a/2)^2))^{\frac{3}{2}}}\right]+\left[\frac{(z+a/2)}{(x^2+y^2+(z+a/2)^2))^{\frac{3}{2}}}\right]\right)}{da}\right)$$

which equals zero. The next term gives

$$q\frac{\cos\vartheta\left(3-5\cos^2\vartheta\right)}{8r^4}a^3$$

and so it goes.

We note in passing that Maple addresses Legendre polynomials using the "with(orthopoly)" command.