252(5): Evaluation of E_1 of Eq. (17) Note 252(4)

The integral to be evaluated is:

$$E_1 = \frac{3e^2\hbar}{16m^2c^2\epsilon_0\pi}\,\underline{\sigma}\cdot\underline{L}\int\frac{\phi^*\phi}{r^3}\,d\tau \quad -(1)$$

where

$$\phi = R_{nl}(r)\,Y_{lm_l}(\theta,\phi) \quad -(2)$$

are the hydrogenic wavefunctions.

The integral is:

$$E_1 = \frac{3e^2\hbar}{16\pi m^2c^2\epsilon_0}\,\underline{\sigma}\cdot\underline{L}\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}\int_{r=0}^{\infty}\frac{R_{nl}^2\,YY^*\,r^2\sin\theta\,dr\,d\theta\,d\phi}{r^3}$$

$$= \frac{3e^2\hbar}{16m^2c^2\epsilon_0\pi}\,\underline{\sigma}\cdot\underline{L}\int_0^\infty\frac{R_{nl}^2r^2}{r^3}\,dr\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}YY^*\sin\theta\,d\theta\,d\phi \quad -(3)$$

in which:

$$\left\langle\frac{1}{r^3}\right\rangle = \int_0^\infty\frac{R_{nl}^2r^2\,dr}{r^3} = \left(\frac{Z}{a_0}\right)^3\frac{1}{n^3\,l\left(l+\frac{1}{2}\right)(l+1)} \quad -(4)$$

where:

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} \quad -(5)$$

is the Bohr radius. Therefore:

$$E_1 = \frac{3e^2\hbar^2}{16m^2c^2\epsilon_0\pi}\left(\frac{Z}{a_0}\right)^3\frac{\underline{\sigma}\cdot\underline{L}}{n^3\,l\left(l+\frac{1}{2}\right)(l+1)}\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}YY^*\sin\theta\,d\theta\,d\phi \quad -(6)$$

2) It is seen that E_1 diverges for S orbitals ($\ell = 0$), but is otherwise finite. This is exactly the same as the result found by Dr. Horst Eckardt by numerical integration.
