252(6): Evaluation of Hamiltonians

Consider the Hamiltonian:

$$\hat{H}\phi = \frac{e}{4m^2c^2}\left(\underline{r}\cdot\underline{p}+i\underline{\sigma}\cdot\underline{L}\right)\frac{\phi}{r^2}\left(\underline{r}\cdot\underline{p}+i\underline{\sigma}\cdot\underline{L}\right)\psi \quad -(1)$$

which is the sum of the following four Hamiltonians:

$$\hat{H}_1\psi = \frac{e}{4m^2c^2}\,\underline{r}\cdot\underline{p}\left(\frac{\phi}{r^2}\,\underline{r}\cdot\underline{p}\,\psi\right) \quad -(2)$$

$$\hat{H}_2\psi = \frac{ie}{4m^2c^2}\,\underline{\sigma}\cdot\underline{L}\left(\frac{\phi}{r^2}\,\underline{r}\cdot\underline{p}\,\psi\right) \quad -(3)$$

$$\hat{H}_3\psi = -\frac{e}{4m^2c^2}\,\underline{\sigma}\cdot\underline{L}\left(\frac{\phi}{r^2}\,\underline{\sigma}\cdot\underline{L}\,\psi\right) \quad -(4)$$

$$\hat{H}_4\psi = -\frac{e}{4m^2c^2}\,\underline{\sigma}\cdot\underline{L}\left(\frac{\phi}{r^2}\,\underline{\sigma}\cdot\underline{L}\,\psi\right) \quad -(5)$$

The Hamiltonian $\hat{H}_1$ was evaluated in notes 252(4) and 252(5). This note evaluates Hamiltonian $\hat{H}_4$:

$$\hat{H}_4\psi = -\frac{e}{4m^2c^2}\,\frac{\phi}{r^2}\,\underline{\sigma}\cdot\underline{L}\,\underline{\sigma}\cdot\underline{L}\,\psi \quad -(6)$$

Note that:

$$\underline{\sigma}\cdot\underline{L}\,\underline{\sigma}\cdot\underline{L} = L^2 + i\underline{\sigma}\cdot\underline{L}\times\underline{L} \quad -(7)$$

where L is an operator. So:

2)

$$\underline{L} \times \underline{L} = i\hbar \underline{L} \quad -(8)$$

and

$$\underline{\sigma} \cdot \underline{L} \, \underline{\sigma} \cdot \underline{L} = L^2 - \hbar \underline{\sigma} \cdot \underline{L} \quad -(9)$$

wet

$$\underline{S} = \frac{1}{2} \hbar \underline{\sigma} \quad -(10)$$

Therefore

$$\underline{\sigma} \cdot \underline{L} \, \underline{\sigma} \cdot \underline{L} = L^2 - 2 \, \underline{S} \cdot \underline{L} \quad -(11)$$

where

$$L^2 \psi = \hbar^2 \ell(\ell+1) \psi \quad -(12)$$

$$\underline{S} \cdot \underline{L} \psi = \frac{\hbar^2}{2} \left(j(j+1) - \ell(\ell+1) - s(s+1) \right) \psi \quad -(13)$$

So:

$$\underline{\sigma} \cdot \underline{L} \, \underline{\sigma} \cdot \underline{L} \psi = \hbar^2 \left(\ell(\ell+1) - j(j+1) + \ell(\ell+1) + s(s+1) \right) \psi$$

$$= \hbar^2 \left(2\ell(\ell+1) - j(j+1) + s(s+1) \right) \psi \quad -(14)$$

Therefore:

$$+\psi = \frac{-e\hbar^2 \phi}{4m^2c^2r^2} \left(2\ell(\ell+1) - j(j+1) + s(s+1) \right) \psi \quad -(15)$$

If it is assumed that:

3)

$$\phi = -\frac{e}{4\pi r \epsilon_0} \quad -(16)$$

then:

$$\boxed{\hat{H}_4 \psi = \frac{e^2 \hbar^2}{16\pi \epsilon_0 m^2 c^2 r^3} \left(2l(l+1) - j(j+1) + s(s+1) \right) \psi}$$

$-(17)$

The energy expectation value using note 252(5) are:

$$E_4 = \frac{e^2 \hbar^2 \left(2l(l+1) - j(j+1) + s(s+1) \right)}{16\pi \epsilon_0 m^2 c^2} \int \frac{\psi^* \psi}{r^3} \, d\tau \quad -(18)$$

where:

$$\int \frac{\psi \psi^*}{r^3} \, d\tau = \left\langle \frac{1}{r^3} \right\rangle \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} Y Y^* \sin\theta \, d\theta \, d\phi \quad -(19)$$

where:

$$\left\langle \frac{1}{r^3} \right\rangle = \int_0^\infty \frac{R_{nl}^2 r^2}{r^3} \, dr = \left(\frac{Z}{a_0} \right)^3 \frac{1}{n^3 l(l+1/2)(l+1)} \quad -(20)$$

and the Bohr radius is:

$$a_0 = \frac{4\pi \epsilon_0 \hbar^2}{m e^2} \quad -(21)$$

The expectation values can be worked out with computer algebra and are completely new and original.