331(4): Testing the Operator Approximation

We wish to work out the expectation value:

$$\left\langle \frac{p_0^2}{2m} L_Z \right\rangle = \int \psi^* \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \frac{\hbar}{i} \frac{\partial}{\partial \phi} \psi \, d\tau$$

$$= \frac{\hbar^3}{2m} \int \psi^* \nabla^2 \frac{\partial}{\partial \phi} \psi \, d\tau \quad — (1)$$

for the hydrogenic wavefunctions. Eq (1) can be compared with the approximation:

$$\left\langle \frac{p_0^2}{2m} L_Z \right\rangle = \left\langle \frac{p_0^2}{2m} \right\rangle \left\langle L_Z \right\rangle$$

$$= -\frac{\hbar^2}{2m} \int \psi^* \nabla^2 \psi \, d\tau \, \frac{\hbar}{i} \int \psi^* \frac{\partial \psi}{\partial \phi} d\tau$$

$$= \frac{i\hbar^3}{2m} \int \psi^* \nabla^2 \psi \, d\tau \int \psi^* \frac{\partial \psi}{\partial \phi} d\tau \quad — (2)$$

The basic operator is:

$$\frac{p_0^2}{2m} L_Z \psi = -\frac{\hbar^2 \nabla^2}{2m} (L_Z \psi) \quad — (3)$$

in which:

$$\nabla^2 (L_Z \psi) = L_Z \nabla^2 \psi + 2 \underline{\nabla} \psi \cdot \underline{\nabla} L_Z + \psi \nabla^2 L_Z \quad - (4)$$

So

$$\int \psi^* \nabla^2 (L_Z \psi) \, d\tau = \int \psi^* L_Z \nabla^2 \psi \, d\tau + 2 \int \psi^* \underline{\nabla} L_Z \cdot \underline{\nabla} \psi \, d\tau + \int \psi^* \nabla^2 L_Z \psi \, d\tau \quad - (5)$$

Here

$$L_Z \psi = \hbar m_L \psi \quad - (6)$$

Using the classical L_Z in eq. (5):

$$\int \psi^* \nabla^2 (L_Z \psi) \, d\tau = L_Z \int \psi^* \nabla^2 \psi \, d\tau + 2 \underline{\nabla} L_Z \cdot \int \psi^* \underline{\nabla} \psi \, d\tau + \nabla^2 L_Z \int \psi^* \psi \, d\tau \quad - (7)$$

The approximation used in previous notes is:

$$\underline{\nabla} L_Z \sim 0 \quad - (8)$$

In the operator representation:

$$\underline{\nabla} (L_Z \psi) = \underline{\nabla} (m_L \hbar \psi) \quad - (9)$$

$$= m_L \hbar \underline{\nabla} \psi$$

$$\neq 0$$

3) So there are additional terms to be considered.
This leads to a very rich spectrum.
The rigorously correct expectation value is:

$$\left\langle \frac{p_0^2}{2m} L_z \right\rangle = \frac{\hbar^3}{2m} \int \psi^* \nabla^2 \left(\frac{\partial \psi}{\partial \phi} \right) d\tau \quad -(10)$$
