Aug 2008

Problem 6: Hydrogen Atom (10 Points)

The spatial component of the ground state wavefunction for the hydrogen atom is

$$\phi(r, \theta, \phi) = Ae^{-\left(\frac{r}{a_o}\right)}$$

where A and a_o (the Bohr radius) are constants.

a) Find A by normalizing the wavefunction. Express your answer in terms of a_o. **(2 Points)**

b) Calculate the expectation value of the potential energy. **(2 Points)**

c) Calculate the expectation value of r and the most probable value for r. **(2 Points)**

d) What is the expectation value for L, the magnitude of the angular momentum? How does this value compare to the prediction of the Bohr model? **(2 Points)**

e) Many solutions to the Schrodinger equation for the hydrogen atom are related to a z-axis despite the fact that the potential energy is spherically symmetric. What defines the z-axis? Explain your answer. **(2 Points)**

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Quantum #6

a) $\psi(r,\theta,\varphi) = A e^{-(r/a_0)}$

$$1 = A^2 \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta\, d\theta\, e^{-(2r/a_0)}$$

$$1 = 4\pi A^2 \int_0^\infty r^2 e^{-2r/a_0}$$

$$\text{* but } \int_0^\infty x^n e^{-ax} dx = \frac{\Gamma(n+1)}{a^{n+1}} \qquad \begin{matrix} x = r \\ n = 2 \end{matrix} \qquad a = 2/a_0$$

$$1 = 4\pi\, \Gamma(3)\, a_0^3 \cdot \tfrac{1}{8} A^2 \qquad (\Gamma(3) = 2)$$

$$\hookrightarrow A = \sqrt{\frac{1}{\pi a_0^3}}$$

b) For the hydrogen atom: $V = \dfrac{-e^2}{4\pi\epsilon_0 r}$

$$\langle\psi|V|\psi\rangle = \int d\vec{r}^{\,3}\, \psi^* V \psi$$

$$= \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta\, d\theta \, \frac{-e^2}{4\pi\epsilon_0 r} e^{-2r/a_0} \cdot \frac{1}{\pi a_0^3}$$

$$= 4\pi \cdot \frac{-e^2}{4\pi\epsilon_0} \int_0^\infty r\, e^{-2r/a_0} dr \qquad \begin{matrix} x = r \\ n = 1 \end{matrix} \qquad a = 2/a_0$$

$$= \frac{-e^2}{\epsilon_0} \frac{\Gamma(2)}{(2/a_0)^2} \cdot \frac{1}{\pi a_0^3}$$

$$= \frac{-e^2 a_0^2}{4\epsilon_0} \cancelto{1}{\Gamma(2)} \cdot \frac{1}{\pi a_0^3}$$

$$= \frac{-e^2}{4\pi\epsilon_0 a_0}$$

c) $$\langle r\rangle = \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta\, d\theta\; r\, e^{-2r/a_0} \cdot \frac{1}{\pi a_0^3}$$

$$= \frac{4}{a_0^3} \int_0^\infty r^3 e^{-2r/a_0} \qquad \begin{matrix} x = r \\ n = 3 \end{matrix} \qquad a = 2/a_0$$

$$= \frac{4}{a_0^3} \frac{\Gamma(4)}{(2/a_0)^4}$$

$$= \frac{4a_0}{16} 3!$$

$$= \frac{6a_0}{4} = \frac{3a_0}{2}$$

#6 (cont.)

c) $\langle\psi|\psi\rangle = \int_0^\infty 4\pi r^2 e^{-2r/a_0}\, dr = P$

$$\frac{dP}{dr} = 0 = \frac{4}{a_0^3} r^2 e^{-2r/a_0}$$

$$\frac{d^2P}{dr^2} = \frac{4}{a_0^3}\left[2re^{-2r/a_0} + r^2 \frac{-2}{a_0} e^{-2r/a_0}\right] = 0$$

* 2nd derivative gives inflection points

$$2r + r^2 \frac{-2}{a_0} = 0$$

$$2 + r\frac{-2}{a_0} = 0$$

$$\frac{-2r}{a_0} = 2$$

$$r = a_0$$

d) $L|nlm\rangle = l(l+1)\hbar^2|nlm\rangle$

* since ground state $|\psi\rangle = |1,0,0\rangle$

$L|1,0,0\rangle = 0$

e) z-axis is defined by the line ⊥ to the plane in which the ground state election orbits the central nucleus.