Problem 6: Hydrogen Atom Measurements

Consider a hydrogen atom, ignoring the spin of the electron, with the usual eigenstates of H, L^2, and L_z written as $|n, \ell, m_z\rangle$.

(a) [2 pts] If the hydrogen atom is in its ground state, $|1, 0, 0\rangle$, what is $\langle r\rangle$, the average distance of the electron from the proton?

(b) [3 pts] If the hydrogen atom is in its ground state, $|1, 0, 0\rangle$, what is the probability of measuring the electron's position to be in the classically forbidden region of space?

The forbidden region is where the energy of the atom is less than the potential energy, $V(r)$, corresponding to a negative value for the classical kinetic energy.

(c) [2 pts] Consider the first excited states of the atom with $\ell = 1$, $|2, 1, m\rangle$. Calculate the expectation value $\langle z\rangle$ for these states (where $z = r\cos\theta$ using standard spherical coordinates).

(d) [3 pts] The state $|2, l, 0\rangle$ has a rather different shape from the states $|2, 1, \pm 1\rangle$. This can be seen by considering the spread in z, $\Delta z = \sqrt{\langle z^2\rangle - \langle z\rangle^2}$, or the expectation value $\langle z^2\rangle$.

Compute the ratio of $\langle z^2\rangle$ in the state $|2, 1, 0\rangle$ to that in the state $|2, 1, 1\rangle$,

$$\frac{\langle z^2\rangle_{2,1,0}}{\langle z^2\rangle_{2,1,1}} \tag{1}$$

Hydrogen Atom States:

$$V(r) = -\frac{e^2}{r}, \quad a_0 = \frac{\hbar^2}{me^2}, \quad Ryd = \frac{e^2}{2a_0}, \quad \alpha = \frac{e^2}{\hbar c} \tag{2}$$

The spatial representation of the Hydrogen Atom energy eigenstates can be written:

$$\psi_{n,\ell,m}(r) = R_{n,\ell}(r)Y_{\ell,m}(\theta,\phi), \quad E_n = -\frac{Ryd}{n^2}$$

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}, \quad Y_{1,0} = \sqrt{\frac{3}{4\pi}}cos\theta, \quad Y_{1,\pm1} = \mp\sqrt{\frac{3}{8\pi}}sin\theta\ e^{\pm i\phi}$$

$$R_{10} = \frac{2}{(a_0)^{3/2}}e^{-r/a_0}, \quad R_{20} = \frac{2}{(2a_0)^{3/2}}\left(1 - \frac{r}{2a_0}\right)e^{-r/2a_0}, \quad R_{21} = \frac{1}{(2a_0)^{3/2}}\frac{r}{\sqrt{3}a_0}e^{-r/2a_0}$$

A possibly useful integral:

$$\int_x^\infty t^n e^{-\alpha t}dt = \frac{n!}{\alpha^{n+1}}\ e^{-\alpha x}\sum_{k=0}^{n}\frac{(\alpha x)^k}{k!}$$

where α is real and positive.

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Quantum #6

a) $\langle r \rangle = \langle 1,0,0 | r | 1,0,0 \rangle$

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

$$= \int_0^{\infty} \frac{4}{a_0^3} r^3 e^{-2r/a_0} dr$$

$$= \frac{4}{a_0^3}\left(\frac{3!}{(2/a_0)^4}\right)$$

$$= \frac{a_0 \cdot 3 \cdot 2}{2^4}$$

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

b) We must determine what the forbidden region is

$$E < V(r)$$

$$\frac{-e^2/2a_0}{n^2} < \frac{-e^2}{r}$$

$$r > 2a_0 n^2$$

$\Rightarrow$ Our problem is the same as above except $r \in [0, \infty)$ now is $r \in [2a_0, \infty)$

$\hookrightarrow$ $$P = \int_{2a_0}^{\infty} \frac{4}{a_0^3} r^2 e^{-2r/a_0} dr$$

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

$$= \frac{4}{a_0^3}\left(\frac{2!}{(2/a_0)^3} e^{-2/a_0 \cdot 2a_0} \sum_{k=0}^{2} \frac{((2/a_0)\cdot 2a_0)^k}{k!}\right)$$

$$= e^{-4}\left[\frac{1}{0!} + \frac{4}{1!} + \frac{16}{2!}\right]$$

$$1 + 4 + 8$$

$$= 13e^{-4}$$

#6(cont.)

c) Our first excited states are $|2,1,m\rangle$

$\hookrightarrow$ $$|2,1,0\rangle = \frac{1}{(2a_0)^{3/2}}\frac{r}{\sqrt{3}a_0}e^{-r/2a_0}\sqrt{\frac{3}{4\pi}}\cos\theta$$

$$|2,1,1\rangle = \frac{-1}{(2a_0)^{3/2}}\frac{r}{\sqrt{3}a_0}e^{-r/2a_0}\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi}$$

$$|2,1,-1\rangle = \frac{1}{(2a_0)^{3/2}}\frac{r}{\sqrt{3}a_0}e^{-r/2a_0}\sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\varphi}$$

* For the $|2,1,0\rangle$ state:

$$\langle z\rangle = \int_0^\infty r^2 dr\int_0^{2\pi}d\varphi\int_0^\pi \sin\theta d\theta \cdot r\cos\theta\cdot\frac{1}{(2a_0)^3}\frac{r^2}{\cancel{3}a_0^2}e^{-r/a_0}\frac{\cancel{3}}{4\pi}\cos^2\theta$$

$$= \int_0^\infty \frac{1}{32\pi a_0^5}r^4e^{-r/a_0}\int_0^{2\pi}d\varphi\int_0^\pi \cos^3\theta\sin\theta d\theta$$

$$= \int_0^\infty dr\frac{1}{16a_0^5}r^4e^{-r/a_0}\int_0^\pi -\cos^3\theta\, d(\cos\theta)$$

$$= \int_0^\infty dr\frac{1}{16a_0^5}r^4e^{-r/a_0}\left[-\frac{1}{4}\cos^4\theta\Big|_0^\pi\right]$$

$$= \int_0^\infty \frac{1}{16a_0^5}r^4e^{-r/a_0}dr\left[\underbrace{-\frac{1}{4}--\frac{1}{4}}_{0}\right]$$

$$= 0$$

* For the $|2,1,1\rangle$ state:

$$\langle z\rangle = \int_0^\infty r^2 dr\int_0^{2\pi}d\varphi\int_0^\pi \sin\theta d\theta\cdot r\cos\theta\cdot\left(\frac{-1}{(2a_0)^3}\right)\frac{r^2}{3a_0^2}e^{-r/a_0}\frac{3}{8\pi}\sin^2\theta e^{i\varphi}$$

$$= \int_0^\infty \frac{-1}{64\pi a_0^5}r^4e^{-r/a_0}dr\int_0^{2\pi}e^{i\varphi}d\varphi\int_0^\pi \sin^3\theta\cos\theta d\theta$$

$$= \qquad\qquad \cdot\, 0$$

$$= 0$$

* The θ is the same in the $|2,1,-1\rangle$ state

$\hookrightarrow$ $\langle z\rangle_{2,1,-1} = 0$

#6 (cont.)

d) * Repeating part c now for $\langle z^2 \rangle$

* For the $|2,1,0\rangle$ state, r and θ integrals change

$$\langle z^2 \rangle = \int_0^\infty \frac{1}{16 a_0^5} r^5 e^{-r/a_0} dr \int_0^\pi \cos^4(\theta) \sin\theta \, d\theta$$

$$= \int_0^\infty \frac{1}{16a_0^5} r^5 e^{-r/a_0} dr \left[-\frac{1}{5}\cos^5(\theta) \Big|_0^\pi \right]$$

$$= \int_0^\infty \frac{1}{16a_0^5} r^5 e^{-r/a_0} dr \cdot \left(-\frac{1}{5}(-1)^5 - -\frac{1}{5}(1)^5 \right)$$

$$= \frac{2}{80 a_0^5} \int_0^\infty r^5 e^{-r/a_0} dr$$

$$= \frac{1}{40a_0^5} \left[\frac{5!}{(2/a_0)^6} \right]$$

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

* For the $|2,1,1\rangle$ state, r, θ integrals change, same as $|2,1,-1\rangle$ state

$$\langle z^2 \rangle = \int_0^\infty \frac{-1}{64\pi a_0^5} r^5 e^{-r/a_0} dr \int_0^{2\pi} \cancel{e^{-i\varphi} e^{i\varphi}} \, d\varphi \int_0^\pi \sin^3\theta \cos^2\theta \, d\theta$$

$$= \frac{-1}{32 a_0^5} \left[\frac{5!}{(2/a_0)^6} \right] \int_0^\pi \sin^3\theta - \sin^5\theta \, d\theta$$

$$= \frac{1}{32 a_0^5} \left(\frac{120 a_0^6}{2^6} \right) \cdot \frac{4}{15} \text{ (from mathematica)}$$

$$= \frac{a_0}{64}$$