

5-2010

### PROBLEM 6: Hyperfine Splitting

The hyperfine splitting in hydrogen comes from a spin-spin interaction between the electron and the proton. The total Hamiltonian can be written as

$$H = \frac{P_p^2}{2m_p} + \frac{P_e^2}{2m_e} - \frac{e^2}{r} + H_{HF}$$

where  $H_{HF} = A \vec{S}_e \cdot \vec{S}_p$ , and  $A$  is a real constant.

- (a) [1 points] What are the spin quantum numbers  $s$  and  $m_s$  of the electron?
- (b) [1 points] What are the spin quantum numbers  $s$  and  $m_s$  of the proton?
- (c) [1 points] What are the spin quantum numbers  $s$  and  $m_s$  of the combined electron-proton system?
- (d) [5 points] Diagonalize  $H_{HF}$  in the total  $\vec{S} = \vec{S}_e + \vec{S}_p$  basis and compute the energy eigenvalues.
- (e) [2 points] Write an expression for the energy of a photon that would be emitted from a hyperfine transition in terms of  $A$ ,  $\hbar$ , and any other relevant constants.

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①

⑥ ①

$$\boxed{S_e = \frac{1}{2}} \\ \boxed{m_s = \pm \frac{1}{2}}$$

②

$$\boxed{S_p = \frac{1}{2}} \\ \boxed{m_s = \pm \frac{1}{2}}$$

③ ~~HF~~  $|S_e - S_p| \leq S \leq S_e + S_p$

$$\boxed{S = 0, 1}$$

$$m_s = m_p + m_e = \cancel{1, 0, -1}$$

$$\boxed{1, 0, -1 = m_s}$$

④  $H_{HF} = A (\vec{S}_e \cdot \vec{S}_p)$

$$(S_e + S_p)^2 = S_e^2 + S_p^2 + 2 S_e \cdot S_p = S^2$$

$$\rightarrow \cancel{HF} S_e \cdot S_p = (S^2 - S_e^2 - S_p^2) \frac{1}{2}$$

basis opms =  $|S_p m_p S_e m_e\rangle$

$$\boxed{|S m S_e S_p\rangle}$$

~~HF~~

~~HF~~

$$S^2 |S m \frac{1}{2} \frac{1}{2}\rangle = \hbar^2 S(S+1) |S m \frac{1}{2} \frac{1}{2}\rangle$$

$$S_e^2 |S m \frac{1}{2} \frac{1}{2}\rangle = \hbar^2 \frac{3}{4} |S m \frac{1}{2} \frac{1}{2}\rangle \\ = S_p^2 |S m \frac{1}{2} \frac{1}{2}\rangle$$

$$S=1 = 2\hbar^2$$

$$S=0 = 0$$

$$\frac{3}{4} - \frac{3}{4} - \frac{3}{4} = \frac{1}{4} \hbar^2$$

$$= -\frac{3}{4} \hbar^2$$

2

④ Continued

$$H_{HF} \hat{=} A \hbar^2$$

$$\begin{array}{c}
 |5m\rangle \\
 \begin{array}{cccc}
 |11\rangle & |10\rangle & |1-1\rangle & |100\rangle
 \end{array} \\
 \left( \begin{array}{cccc}
 \frac{1}{4} & 0 & 0 & 0 \\
 0 & \frac{1}{4} & 0 & 0 \\
 0 & \cancel{1/4} 0 & \frac{1}{4} & 0 \\
 0 & 0 & 0 & -\frac{3}{4}
 \end{array} \right)
 \end{array}$$

eigenvalues are  $\frac{A\hbar^2}{4}$  &  $-\frac{3\hbar^2}{4}$

$\uparrow$                        $\uparrow$   
 degeneracy          degeneracy of  
 of 3                      1

⑤ ~~Answer~~

$$\frac{A\hbar^2}{4} + \frac{3\hbar^2 A}{4} = \boxed{\hbar^2 A}$$

**PROBLEM 2: Hydrogenic Atoms with One Electron**

In terms of the first Bohr radius,  $a_0 \equiv \hbar/(c\alpha m_e)$ , where  $\alpha$  is the fine-structure constant, the ground-state eigenfunction of a hydrogen atom is

$$\psi_{1,0,0}(r, \theta, \varphi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}.$$

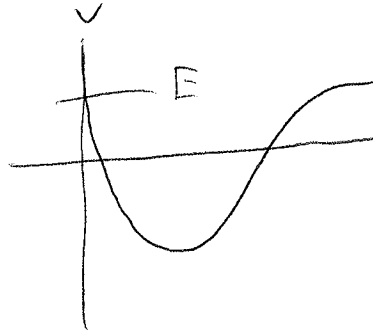
- (a) [3 points] Evaluate the probability of finding an electron in the ground-state of a hydrogen atom in the classically forbidden region. The classically forbidden region is the region of space where the classical kinetic energy is negative.
- (b) [4 points] For the ground state, evaluate the uncertainty in the Cartesian coordinate  $x$  and the uncertainty in the corresponding component of the linear momentum,  $p_x$ . *Hint: You need not use the explicit form of the operator for the linear momentum to evaluate  $\Delta p_x$ .*
- (c) [3 points] Show explicitly that the product of your uncertainties,  $\Delta x \Delta p_x$ , is consistent with the Heisenberg uncertainty principle.

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①

$$\textcircled{2} \psi_{100} = \frac{1}{\sqrt{11}a_0^3} e^{-r/a_0}$$

(A) Classically  $\rightarrow T+V=E \rightarrow T=E-V$  ;  $T$  is + which means  $E > V$



So its where

$$E < V$$

$$E \text{ For Hydrogen is } \frac{-13.6 \text{ eV}}{n^2} = -13.6 \text{ eV}$$

$$E = -\frac{Ryd}{n^2}$$

$$\rightarrow Ryd = \frac{e^2}{2a_0} \quad \text{remember this} \\ \star \star \star \star$$

lets see if you can find it

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dr^2} - \frac{e^2 \psi}{r} = E \psi$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dr^2} - \frac{e^2 \psi}{r} = E \psi$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dr^2} - \frac{e^2 \psi}{r} = E \psi$$

$$\rightarrow \frac{-e^2}{2a_0} < \frac{-e^2}{r} \rightarrow \boxed{r > 2a_0}$$

2

~~Q31~~ (A) 
$$P = \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{1}{\sqrt{a_0^3}} e^{-2r/a_0} r^2 \sin\theta d\phi d\theta dr$$

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

~~$$\frac{4\pi}{a_0^3} \left( \frac{r^3}{3} \right) \Big|_0^\infty$$~~

~~$$\frac{4\pi}{a_0^3}$$~~

$$\frac{e^{-2r/a_0}}{(-2/a_0)} \left( r^2 - \frac{2r}{(-2/a_0)} + \frac{2}{(-2/a_0)^2} \right) \Big|_0^\infty$$

$$= - \left( \frac{e^{-4}}{(-2/a_0)} \left( 4a_0^2 - \frac{4a_0}{(-2/a_0)} + \frac{2}{(-2/a_0)^2} \right) \right)$$

$$= + \frac{e^{-4} a_0}{2} \left( 4a_0^2 + 4a_0^2 + \frac{1}{2} a_0^2 \right)$$

$$= \frac{8}{2} \frac{4}{2} + \frac{1}{2}$$

$$\frac{13 e^{-4} a_0^2}{4}$$

$$\rightarrow P = 13 e^{-4}$$

(B)

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

(3)

~~ANS~~ 
$$\psi = \frac{1}{\sqrt{\pi/a_0^3}} e^{-\sqrt{x^2+y^2+z^2}/a_0}$$
~~ANS~~

~~ANS~~ easier  $\rightarrow$  ~~ANS~~  $x = r \sin \theta \cos \phi$

$$\rightarrow \langle x \rangle = \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{1}{\pi a_0^3} e^{-2r/a_0} r^3 \sin^2 \theta \cos \phi \, dr \, d\phi \, d\theta$$

$$\int_0^{2\pi} \cos \phi \, d\phi = 0$$

$$= 0$$

$$\rightarrow \langle x^2 \rangle = \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{1}{\pi a_0^3} e^{-2r/a_0} r^4 \sin^3 \theta \cos^2 \phi \, dr \, d\phi \, d\theta$$

$$\int_0^{2\pi} \cos^2 \phi \, d\phi$$

$$= \frac{2\pi}{2} = \pi$$

$$\rightarrow \int_0^\pi \sin^3 \theta \, d\theta = -\frac{\cos \theta}{1} + \frac{\cos^3 \theta}{3} \Big|_0^\pi$$

$$= \left(1 - \frac{1}{3}\right) + \left(+1 + \frac{1}{3}\right)$$

$$= \frac{2}{3} + \frac{2}{3} = \frac{4}{3}$$

(B) Continued

(4)

$$\frac{4}{3} \sqrt{\pi} \frac{1}{\sqrt{\pi} a_0^3} \int_0^\infty e^{-2r/a_0} r^4 dr$$

$$= \frac{4}{3} \sqrt{\pi} \frac{1}{\sqrt{\pi} a_0^3} \frac{24}{32} \frac{a_0^5}{32}$$

$$\frac{\Gamma(4+1)}{(2/a_0)^5} = 4 \cdot 3 \cdot 2 \cdot 1 = 24$$

$$\begin{matrix} 2 & 2 & 2 & 2 & 2 \\ 4 & 8 & 16 & 32 \end{matrix}$$

$$\frac{4}{3} a_0^5 \frac{3}{4}$$

$$= a_0^2$$

→ ~~dx~~ ~~dt~~

$$\boxed{\Delta x = a_0}$$

$$\underline{P_x} = -i\hbar \frac{\partial}{\partial x}$$

$$\frac{\partial}{\partial x} e^{-\sqrt{x^2+y^2+z^2}/a_0}$$

$$\frac{1}{2} - \frac{3}{2}$$

$$U = \sqrt{x^2+y^2+z^2}$$

$$\frac{dU}{dx} = \frac{x}{\sqrt{x^2+y^2+z^2}} = \frac{x}{r} = \cos\phi \cos\theta$$

~~dx~~

$$\frac{de^{-U/a_0}}{dU} = -a_0 e^{-U/a_0}$$

$$\langle P_x \rangle = 0 \text{ since } \int = 0$$



$$\frac{\partial^2}{\partial x^2} e^{-r/a_0} = -a_0 \cos\theta \sin\theta \frac{\partial}{\partial x} e^{-r/a_0} = a_0^2 \cos^2\theta \sin^2\theta \quad (5)$$

$$\rightarrow \langle p_x^2 \rangle = \frac{\hbar^2}{3} \frac{4\pi}{4\pi a_0^3} a_0^2 \int_0^\infty e^{-2r/a_0} r^2 dr$$

$$\frac{\Gamma(2+1)}{(2/a_0)^3}$$

$$= \hbar^2 \frac{4(2)}{3 a_0^3} a_0^3 = \frac{1}{3} a_0^2 \hbar^2$$

$$p^2 = k_9 \frac{m^2}{s^2}$$

$$\hbar = k_9 \frac{m^2}{s} = k_9 \frac{m^2}{s^2}$$

you're very close, This is how to

do it but the

Math is wrong,

someone here

F-2015

### 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  $|2, 1, 0\rangle$  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  $|2, 1, 1\rangle$ ,

$$\frac{\langle z^2 \rangle_{2,1,0}}{\langle z^2 \rangle_{2,1,1}} \quad (1)$$

Hydrogen Atom States:

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

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

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

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

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

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  $\alpha$  is real and positive.

$$\textcircled{C} |n, l, m_l\rangle$$

$$\textcircled{A} |1, 0, 0\rangle = R_{1,0} Y_{0,0}$$

$$= \frac{2}{(a_0)^{3/2}} e^{-r/a_0} \frac{1}{\sqrt{4\pi}}$$

→ ~~mean~~ average = expectation value

$$\rightarrow \langle r \rangle = \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{4}{a_0^3} e^{-2r/a_0} \frac{1}{\sqrt{4\pi}} r r^2 \sin\theta dr d\theta d\phi$$

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

$$\frac{\Gamma(3+1)}{\left(\frac{2}{a_0}\right)^4} = \frac{6 a_0^4}{16}$$

$$= \boxed{\frac{3}{2} a_0 = \langle r \rangle}$$

$$\textcircled{B} -\frac{e^2}{r} > -\frac{e^2}{2a_0 n^2} \rightarrow \boxed{2a_0 < r}$$

↑

Multiply both sides by  $(-1)$

→ multiply or divide

- #'s in inequality → Flip

(B) Continued

(2)

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

$$\frac{13}{26}$$

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

$$\frac{16}{64}$$

$$1 + 4 + \frac{16}{2}$$

$$= 13$$

$$= \frac{4 \cdot 26}{4 \cdot 2} e^{-4/a_0}$$

$$= \boxed{13 e^{-4/a_0} = P}$$

(C)  $|2, 1, m\rangle = R_{2,1} Y_1^m$

$$m=0 \rightarrow R_{2,1} Y_1^0 = \frac{1}{(2a_0)^{3/2}} \frac{r}{\sqrt{3} a_0} e^{-r/2a_0} \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$\rightarrow z = r \cos\theta$$

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

Continued

3

This will be  $\int_0^\pi \cos^3 \theta \sin \theta d\theta = 0$

$$= \cancel{\frac{1}{2}} \frac{1}{8} \frac{R_0^3}{a_0^2} \int_0^\infty e^{-r/a_0} r^4 \int_0^\pi \cos^3 \theta \sin \theta d\theta$$

$$u = \cos \theta$$

$$\frac{du}{d\theta} = -\sin \theta$$

$$\int_0^\pi u^3 du = \frac{1}{4} u^4 \Big|_0^\pi = 0$$

$$\rightarrow \langle L_z \rangle_{210} = 0$$

$$\cancel{R_{21}} V_{\pm}^{\pm 1} = \frac{1}{(2a_0)^{3/2}} \frac{r}{\sqrt{3} a_0} e^{-r/2a_0} \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}$$

$$\langle L_z \rangle_{\pm} = \frac{1}{(2a_0)^3} \frac{1}{3} \frac{1}{a_0} \frac{3}{8\pi} \int_0^\infty r^5 e^{-r/2a_0} dr \int_0^\pi \cos \theta \sin^3 \theta d\theta \int_0^{2\pi} d\phi$$

$$\langle L_z \rangle_{21\pm 1} = 0$$

(4)

①  $\langle z^2 \rangle_{2,1,0}$

$$= \frac{1}{2} \frac{a_0^3}{8 a_0^2} \int_0^\infty e^{-r/a_0} r^2 r^2 r^2 dr \int_0^\pi \cos^2 \theta \cos^2 \theta \sin \theta d\theta$$

actually

$$\frac{1}{a_0^5}$$

make

mistake

$$\frac{6!}{\left(\frac{1}{a_0}\right)^7}$$

$$u = \cos \theta$$

$$\frac{du}{d\theta} = -\sin \theta$$

$$-\frac{1}{5} \cos^5 \theta \Big|_0^\pi$$

$$-\frac{1}{5} \underbrace{(-1 - 1)}_{-2} = \frac{2}{5}$$

$$= \frac{1}{5} \frac{a_0^{\cancel{2}}}{8} 6!$$

$$\rightarrow \langle z^2 \rangle_{2,1,1} = \frac{1}{8 a_0^5} \frac{7!}{\cancel{8}} \int_0^\infty r^6 e^{-r/a_0} dr \int_0^\pi \cos^2 \theta \sin^3 \theta d\theta$$

$$\frac{6!}{\left(\frac{1}{a_0}\right)^7} \int_0^\pi (1 - \sin^2 \theta) \sin^3 \theta d\theta$$

$$\int_0^\pi \sin^3 \theta d\theta = \int_0^\pi \sin^2 \theta d\theta$$

$$-\cos \theta + \frac{\cos^3 \theta}{3} \Big|_0^\pi$$

$\left(1 - \frac{1}{3}\right) - \left(-1 + \frac{1}{3}\right)$

$$\left(1 - \frac{1}{3}\right) - \left(-1 + \frac{1}{3}\right)$$

$$\frac{4}{3} - \frac{2}{3} = \frac{2}{3}$$

$$\left[ -\frac{\sin^4 \theta \cos \theta}{5} + \frac{4}{5} \frac{4}{3} \right] \Big|_0^\pi$$

$$\frac{16}{15}$$

$$\rightarrow \frac{20}{15} - \frac{16}{15} = \frac{4}{15}$$

5

① Continued

$$\frac{1}{8a_0^5} \frac{1}{\cancel{4!}} 6! a_0^7 \frac{\cancel{4!}}{15} = 6! \frac{a_0^2}{(8)(15)}$$

$$\rightarrow \frac{\langle r^2 \rangle_{210}}{\langle r^2 \rangle_{211}} = \frac{1}{5} \frac{\cancel{a_0^2}}{\cancel{4!}} \frac{\cancel{4!}}{\cancel{a_0^2}} \frac{1}{\cancel{4!}} \frac{1}{\cancel{a_0^2}} (8)(15)$$

$$= \boxed{3}$$

S-2014

### PROBLEM 5: Zeeman Field

Consider the eight  $n = 2$  states of Hydrogen. This problem is on the *strong* field Zeeman effect with spin-orbit interaction. Assume that the constant magnetic field  $B$  lies along the  $z$ -direction. The spin orbit coupling term is

$$H_{SO} = \frac{1}{2m_l^2 c^2} \frac{1}{r} \frac{dV}{dr} \mathbf{L} \cdot \mathbf{S},$$

where  $V(r)$  is the Coulomb potential,  $c$  is the speed of light and  $m_l$  is the angular momentum projection quantum number. Remember:

$$\langle n, l, m_l | \frac{1}{r^3} | n, l, m_l \rangle = \frac{1}{a_0^3 n^3 l(l + \frac{1}{2})(l + 1)}$$

for  $l \neq 0$ .

- Find a general expression for the energy due to the spin-orbit term in the physical limit of strong magnetic field, where the strong field Zeeman splitting expressions are valid. Express your answer in terms of the good quantum numbers in this problem. Recall that because of the strong magnetic field, the good quantum numbers in this regime are  $n, l, m_l$  and  $m_s$  and not  $j$  and  $m_j$ . (Hint: compute  $\langle H_{SO} \rangle$  in the proper basis) (3 Points)
- Explicitly write down the quantum numbers for all eight  $n = 2$  states. Find the energy of each state under strong field Zeeman splitting. Express the energy of each state as the sum of 3 terms: the Bohr energy, the spin-orbit interaction, and the Zeeman contribution. (4 Points)
- If you ignore the spin-orbit interaction, how many distinct energy levels are there and what are their degeneracies? (3 Points)



①

S-2014⑤  $n=2$  Strong Field Zeeman  $\vec{B} = B \hat{z}$ 

$$H_{SO} = \frac{1}{2m_e^2 c^2} \frac{1}{r} \frac{dV}{dr} \vec{L} \cdot \vec{S}$$

①  $\vec{L} \cdot \vec{S} =$  ~~scribbles~~

$$L_x S_x + L_y S_y + L_z S_z$$

$$L_+ = L_x + iL_y \quad L_- = L_x - iL_y$$

$$\cancel{S_+} S_+ = S_x + iS_y \quad \cancel{S_-} S_- = S_x - iS_y$$

$$\cancel{L_+ S_+} = \cancel{L_x S_x} + \cancel{iL_x S_y} + iL_y S_x - L_y S_y$$

$$\cancel{L_- S_-} = L_x S_x +$$

$$\rightarrow L_+ S_- = L_x S_x - iL_x S_y + iL_y S_x + L_y S_y$$

$$L_- S_+ = L_x S_x + iS_y L_x - iL_y S_x + L_y S_y$$

$$\rightarrow \vec{L} \cdot \vec{S} = \frac{1}{2} (L_+ S_- + L_- S_+)$$

(2)

(A) Continued

good quantum #'s are  $n, l, m_l, m_s$ 

$$V = \frac{k}{r} \quad \frac{dV}{dr} = -\frac{k}{r^2}$$

$$\rightarrow H_{SO} = \frac{-k}{4m_l^2 c^2} \frac{1}{r^3} (L_+ S_- + L_- S_+ + 2L_z S_z)$$

give  $\phi$

$$\rightarrow \langle n, l, m_l, m_s | H_{SO} | n, l, m_l, m_s \rangle$$

$$= -\frac{k}{2m_l^2 c^2} \langle n, l, m_l, m_s | \frac{L_z S_z}{r^3} | n, l, m_l, m_s \rangle$$

$$= -\frac{m_s k \hbar^2}{2m_l c^2} \langle n, l, m_l, m_s | \frac{1}{r^3} | n, l, m_l, m_s \rangle$$

$$\frac{1}{a_0^3 n^3 l(l+\frac{1}{2})(l+1)}$$

$$\rightarrow \Delta E_{SO} = \frac{-m_s k \hbar^2}{2m_l c^2 a_0^3 n^3 l(l+\frac{1}{2})(l+1)}$$

Technically a  
perturbation.

(B)	$n=2$	$l=0$	$m_l=0$	$m_s = \frac{1}{2}$
	2	0	0	$-\frac{1}{2}$
	2	1	-1	$\frac{1}{2}$
	2	1	-1	$-\frac{1}{2}$
	2	1	0	$\frac{1}{2}$
	2	1	0	$-\frac{1}{2}$

③ Continued

$$\begin{array}{cccc} 2 & 1 & 1 & \frac{1}{2} \\ 2 & 1 & 1 & -\frac{1}{2} \end{array}$$

Weak Field  $\rightarrow E_{\text{Zeeman}} = \mu_B m_j B$

Bohr  
mag

Strong Field  $\Rightarrow E_{\text{Zeeman}} = \mu_B (m_l + 2m_s) B$

Bohr energy  $= - \frac{13.6 \text{ eV}}{n^2}$

~~But~~ Simply add all these

③  $E_B + E_Z$

~~$l=0$   $m_s = \frac{1}{2}$   $E_B - \mu_B B$~~   
 ~~$l=0$   $m_s = -\frac{1}{2}$   $E_B + \mu_B B$~~   
 ~~$l=1$   $m_s = -$~~

Should be  
Simple

$E_B + E_Z$

$l=0$   
 $l=1$   $m_l = -1, 0, 1$   
 $m_l = \pm \frac{1}{2}$  For  $l=1$

### Problem 4: Properties of the Hydrogen Atom

The wavefunctions for the ground state and first excited states of the hydrogen atom are given on the first page of this test.

- (a) [2 pt] For the ground state of the hydrogen atom, determine the expectation value for the radial position of the electron,  $\langle 1, 0, 0 | r | 1, 0, 0 \rangle$ .

- (b) [3 pt] Define the radial probability density for the electron in a hydrogenic eigenstate:  $P_{n,\ell,m}(r)dr$  as the probability of the electron being measured in the spherical shell between  $r$  and  $r + dr$ .

Write down expressions for  $P_{1,0,0}(r)$  and  $P_{2,1,1}(r)$ , and sketch these as functions of  $r$ .

Hint: Remember that the integral of the probability density over  $r$  must be equal to one,

$$\int_0^\infty P_{n,\ell,m}(r)dr = 1 \quad (1)$$

- (c) [3 pt] For the ground state of the hydrogen atom, determine the most probable radius for the electron. Compare your result to part (a) and explain the similarities and differences.
- (d) [1 pt] What is the functional form for  $P_{1,0,0}(r)$  in the limit as  $r \rightarrow 0$ ? Explain your result considering that the ground state wavefunction is non-zero at  $r = 0$ .
- (e) [1 pt] What are the functional forms of  $P_{1,0,0}(r)$ ,  $P_{2,1,1}(r)$ , and  $P_{200}(r)$  as  $r \rightarrow 0$ ? Explain the similarities and differences.

F-2012

①

$$(4) \quad (A) \quad \langle 1,0,0 | r | 1,0,0 \rangle$$

$$2+2=4+2=6$$

$$\psi_{1,0,0} = \frac{2}{(a_0)^{3/2}} e^{-r/a_0} \frac{1}{\sqrt{4\pi}}$$

$$\Rightarrow \langle 1,0,0 | r | 1,0,0 \rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \cancel{\psi_{1,0,0}} \psi_{1,0,0}^* r \psi_{1,0,0} r^2 \sin\theta dr d\theta d\phi$$

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

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

$$= \frac{4}{a_0^3} \frac{\Gamma(3+1)}{(2/a_0)^{3+1}} = \frac{4}{a_0^3} \frac{3! a_0^4}{2^4}$$

$$= \frac{6 \times 4}{2^4} a_0$$

$$= \frac{24}{16} a_0$$

$$= \frac{12}{8} a_0 = \boxed{\frac{3}{2} a_0}$$

$$\textcircled{B} \quad 1 = A^2 \int_0^\infty \int_0^\pi \int_0^{2\pi} \psi^2 r^2 dr d\theta d\phi$$

$$= 4\pi A^2 \int_0^\infty \psi^2 r^2 dr$$

$$\underline{P_{1,0,0}(r)} \rightarrow \frac{4\pi}{4\pi} A^2 \int_0^\infty \frac{4}{(a_0)^3} e^{-2r/a_0} r^2 dr = 1$$

$$\rightarrow A^2 \frac{4}{(a_0)^3} \frac{\Gamma(2+1)}{(2/a_0)^{2+1}} = 1$$

$$\rightarrow A^2 \frac{4}{(a_0)^3} \frac{2 a_0^2}{2^2} = 1 \rightarrow \underline{A^2 = 1}$$

$$\rightarrow \boxed{P_{1,0,0}(r) = \frac{4}{(a_0)^3} e^{-2r/a_0} r^2 dr}$$

$$\underline{P_{2,1,1}(r)} \rightarrow \int_0^{2\pi} \int_0^\pi \int_0^\infty A^2 \frac{1}{(2a_0)^3} \frac{r^2}{3a_0^2} e^{-r/a_0} \frac{3}{8\pi} \sin^2 \theta r^2 \sin \theta dr d\theta d\phi$$

$$\rightarrow \int_0^\pi \sin^3 \theta d\theta$$

$$= \left( -\cos \theta + \frac{\cos^3 \theta}{3} \right) \Big|_0^\pi$$

$$= \left( 1 - \frac{1}{3} \right) - \left( -1 + \frac{1}{3} \right)$$

$$= 1 + 1 - \frac{1}{3} - \frac{1}{3}$$

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

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

$$\rightarrow \frac{2\pi \left( \frac{4}{3} \right) A^2 \frac{1}{(2a_0)^3} \frac{1}{3a_0^2} \frac{3}{8\pi}}{\Gamma(4+1) a_0^5} \int_0^\infty r^4 e^{-r/a_0} dr = 1$$

$$\Gamma(4+1) a_0^5$$

$$= 4 \times 3 \times 2 \times 1 = 24 a_0^5$$

$$\rightarrow \frac{8 \times 24}{3} A^2 = 1$$

$$\rightarrow 64 A^2 = 1 \rightarrow A = \frac{1}{8}$$

③ Continued

③

$$1 = \frac{1}{64} \frac{1}{\rho a_0^3} \frac{1}{\rho a^2} \frac{\pi}{8} \frac{1}{3} \int_0^{\infty} r^4 e^{-r/a_0} dr$$

= This can't be right since this

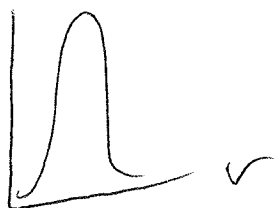
doesn't equal 1

→ has to be  $\frac{1}{24a_0^5} \int_0^{\infty} r^4 e^{-r/a_0} dr$

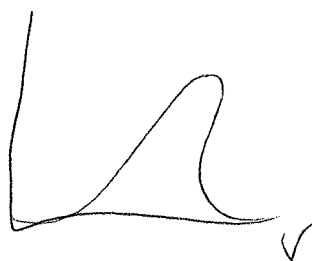
if you run into this

just do  $\int_0^{\infty} r^2 e^{-r/a_0} dr = 1$

$P_{1,0}$



$P_{2,1}$



$$\textcircled{C} \frac{dP}{dr} = 0 \rightarrow \frac{1}{(a_0)^3} \left[ -\frac{2}{a_0} r^2 + 2r e^{2r/a_0} \right] = 0$$

$$\rightarrow r^2 \frac{1}{a_0} = r$$

$$\rightarrow \boxed{r = a_0}$$

③ Continued

④

expectation value is  $\frac{3}{2}a_0 = r$  which is the average measurement from multiple measurements.

The most probable radius is where the probability is at a maximum. The P.d.f has a ~~max~~

tail which spreads the wave.

④  $\lim_{r \rightarrow \infty} P_{1,0,0} = \frac{0}{\infty} = 0$

↳ The probability changes to a point,

⑤  $\lim_{r \rightarrow 0} P_{2,0,0} \rightarrow \left( \frac{2}{(2a_0)^{3/2}} \right)^2$

~~scribbles~~

All 3  $\rightarrow 0$

$P_{2,1,1} \rightarrow 0$

$P_{2,0} \rightarrow \frac{r^2}{2a_0^3} e^{-r/a_0} \left( 1 - \frac{r}{2a_0} \right)^2$

~~scribbles~~  $\frac{r^2}{2a_0^3} e^{-r/a_0} \left( 1 - \frac{r}{2a_0} \right)^2$

$\rightarrow 0$



## Problem 6: The hydrogen atom (10 points)

7

209

The figure below shows the radial function  $R_{n,\ell}(r)$  for a stationary state of atomic hydrogen. The normalized Hamiltonian eigenfunction for this state, in atomic units, is

$$\psi_{n,\ell,m_\ell}(\mathbf{r}) = \frac{1}{81} \sqrt{\frac{2}{\pi}} (6-r) e^{-r/3} \cos \theta. \quad (1)$$

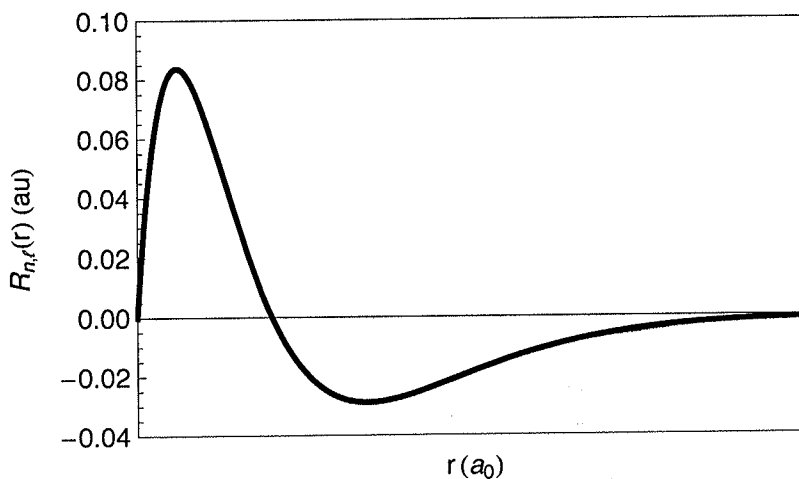


Figure 1: A radial function for a stationary state of atomic hydrogen.

1. **3 points.** What are the values of the quantum numbers  $n$ ,  $\ell$ , and  $m_\ell$  for this state? To receive any credit, you must fully justify your answer.
2. **1 points.** What is the energy (in eV) of this state?
3. **2 points.** What are the mean value and uncertainty in  $r$  (in atomic units) for this state?
4. **2 points.** Calculate the value of  $r$  (in atomic units) at which a position measurement would be most likely to find the electron if the atom is in this state.
5. **2 points.** From Eq. 1, generate the normalized eigenfunction  $\psi_{n,\ell,m_\ell+1}(\mathbf{r})$ .

**Hint:**

$$\int_0^\infty e^{-2r/3} r^n dr = n! \left(\frac{3}{2}\right)^{n+1} \quad (2)$$

**Hint:** The following table gives the orbital-angular-momentum operators in Cartesian and spherical coordinates.

Component	Cartesian coordinates	Spherical coordinates
$\hat{L}_x$	$-i\hbar \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$	$i\hbar \left( \sin \varphi \frac{\partial}{\partial \theta} + \cot \theta \cos \varphi \frac{\partial}{\partial \varphi} \right)$
$\hat{L}_y$	$-i\hbar \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$	$-i\hbar \left( \cos \varphi \frac{\partial}{\partial \theta} - \cot \theta \sin \varphi \frac{\partial}{\partial \varphi} \right)$
$\hat{L}_z$	$-i\hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$	$-i\hbar \frac{\partial}{\partial \varphi}$
$\hat{L}^2$	$\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$	$-\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right]$

Table 1: Components and square of the orbital angular momentum operator in Cartesian and spherical coordinates.

S-2009

①

$$\psi_{n,l,m}(r) = \frac{1}{r} \sqrt{\frac{2}{\pi}} (6-r) e^{-r/3} \cos\theta$$

$$\textcircled{A} \quad L^2 \psi = \hbar^2 l(l+1) \psi$$

$$-\hbar^2 \left[ \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left( \sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \psi$$

$$= -\hbar^2 A \left[ \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (-\sin\theta \cos\theta) \right]$$

$$= -\hbar^2 A \left[ \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (\sin\theta (-\sin\theta)) \right]$$

$$= \hbar^2 A \left[ \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (\sin^2\theta) \right] = \hbar^2 A \left[ \frac{1}{\sin\theta} (2 \cos\theta \sin\theta) \right]$$

$$= 2 A \cancel{\hbar^2} \cos\theta = \hbar^2 l(l+1) A \cos\theta$$

$$l(l+1) = 2$$

$$\boxed{l=1}$$

$$\rightarrow L_z \psi = m\hbar \psi \rightarrow -i\hbar \frac{\partial}{\partial\phi} \psi = \cancel{\phi} \rightarrow \boxed{m=\phi}$$

$$\# \text{ of Nodes} = (n - l - 1) = \cancel{1}$$

$$(n - 2) = \cancel{1}$$

$$\boxed{n=4}$$

$$\boxed{n=3}$$

(B)

$$E = -13.6 \text{ eV} \cdot \frac{1}{9}$$

$$= -13.6 \text{ eV} \cdot \frac{1}{9}$$

(2)

$$E = \frac{-13.6 \text{ eV}}{9}$$

(C)

$$\langle r \rangle = \int_{\text{All space}} r \psi^2 d^3r$$

$$= \frac{1}{81} \left( \frac{2}{\pi} \right) \int_0^\infty \int_0^\pi \int_0^{2\pi} r^3 (6-r) e^{-2r/3} \cos^2 \theta \sin \theta d\phi d\theta dr$$

$$= \frac{1}{81} \left( \frac{2}{\pi} \right) (2\pi) \int_0^\infty \int_0^\pi r^3 (6-r) e^{-2r/3} \cos^2 \theta \sin \theta d\theta dr$$

$$= \frac{1}{81^2} \left( \frac{2}{\pi} \right) \int_0^\infty \int_0^\pi r^3 (6-r)^2 e^{-2r/3} \cos^2 \theta \sin \theta d\theta dr$$

$$= \frac{1}{81^2} (4) \int_0^\infty r^3 (6-r)^2 e^{-2r/3} \cos^2 \theta \sin \theta d\theta dr$$

$$= \frac{1}{81^2} 4 \int_0^\infty r^3 (6-r)^2 e^{-2r/3} \left[ \frac{-\cos^{n+1} \theta}{n+1} \right]_0^\pi$$

$$(6-r)(6-r)$$

$$= 36 - 12r + r^2$$

$$\frac{5 \times 4 \times 3 \times 2 \times 1}{20 \times 3 \times 2 \times 1} = 120$$

$$= -\frac{1}{3} [-1 - 1] = \frac{2}{3}$$

$$= \frac{8}{3(81^2)} \left[ \int_0^\infty 36r^3 e^{-2r/3} dr - \int_0^\infty 12r^4 e^{-2r/3} dr + \int_0^\infty r^5 e^{-2r/3} dr \right] = \frac{2}{3}$$

$$36(6) \left( \frac{3}{2} \right)^4 - 12(24) \left( \frac{3}{2} \right)^5 + 120 \left( \frac{3}{2} \right)^6$$

Continued

$$\begin{array}{r} 3 \\ 36 \\ 6 \\ \hline 216 \end{array}$$

$$3 \times 3 \times 3 \times 3 = 81$$

$$2 \times 2 \times 2 \times 2 = 16$$

3

$$\begin{array}{r} 24 \\ 12 \\ \hline 48 \\ 240 \\ \hline 288 \end{array}$$

$$\begin{array}{r} 81 \\ 3 \\ \hline 243 \end{array}$$

$$\begin{array}{r} 16 \\ 2 \\ \hline 32 \end{array}$$

$$\begin{array}{r} 243 \\ 3 \\ \hline 729 \end{array}$$

$$\begin{array}{r} 132 \\ 2 \\ \hline 264 \end{array}$$

$$= \frac{8}{3(81^2)} \left[ \frac{(216)(81)}{16} - \frac{(288)(243)}{32} + \frac{(120)(729)}{64} \right]$$

$$\begin{array}{r} 216 \\ 81 \\ \hline 216 \\ 2240 \\ \hline 2456 \\ \times 3 \\ \hline 7368 \end{array}$$

$$\begin{array}{r} 266 \\ 243 \\ \hline 11520 \\ 57600 \\ \hline 69120 \end{array}$$

$$\beta_1 = h \quad \beta_2 = h$$

$$\begin{array}{l} \langle r \rangle \\ \sigma(r) = \sqrt{\langle r^2 \rangle - \langle r \rangle^2} \end{array}$$

$$\frac{d(\psi^2)}{dr} = \phi$$

$$L_+ \psi = \sqrt{(l+m)(l-m+1)} \psi_{m+1}$$

HW 5-2008

### Problem 6: Spherically Symmetric States: (10 Points)

Consider eigenfunctions of the Hamiltonian of a particle in a three-dimensional central potential. In particular, consider those eigenfunctions that depend only on the electron's radial coordinate  $r$ , that is  $\Psi_E = \Psi_E(r)$ . States represented by such eigenfunctions are called "spherically symmetric states".

1. Derive an equation for a function  $\chi_E(r)$  defined by:

$$\Psi_n(r) \equiv \frac{1}{r} \chi_n(r),$$

where  $n$  is the principle quantum number. **(2 Points)**

The remainder of this problem concerns a hydrogen atom in the approximation that we neglect all interactions except the Coulomb interaction and treat the proton as an infinitely massive point particle at the origin.

2. Sketch  $\chi_n(r)$  for the lowest three spherical bound states of the hydrogen atom. Justify the qualitative features of each function. **(2 Points)**
3. **(2 Points)**. Consider the eigenfunction for the ground state. Prove that to be physically admissible this function must decay exponentially as  $r$  becomes infinite.

$$\chi_1(r) \rightarrow e^{-\alpha r}, \text{ when } r \rightarrow \infty$$

where  $\alpha$  is a constant, and that therefore  $\chi_1(r)$  must have the form.

$$\chi_1(r) = f(r)e^{-\alpha r}.$$

4. Use  $f(r) = r$ . Justify why this is an appropriate choice and show that the above equation is a solution of the equation you derived for  $\chi_1(r)$  and determine the corresponding eigenvalue  $E_1$ . **(2 Points)**
5. Derive an expression for the constant  $\alpha$  in terms of fundamental constants. **(2 Points)**

S-2008

①

$$\textcircled{b} \left[ -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{r} \right] \psi(\theta, \phi, r) = E(\theta, \phi, r)$$

$$\textcircled{A} \nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2}$$

$$\rightarrow -\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] - \frac{e^2}{r} \psi = E \psi$$

$$\rightarrow L^2 = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$$

$$\rightarrow -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{L^2}{2mr^2} \psi - \frac{e^2}{r} \psi = E \psi$$

$$\rightarrow \psi = \psi_n(r) Y_{ml}(\theta, \phi)$$

$$\rightarrow -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi_n(r)}{\partial r} \right) Y + \frac{L^2 \psi_n Y}{2mr^2} - \frac{e^2}{r} \psi_n Y = E \psi_n Y$$

$$\rightarrow -\frac{\hbar^2}{2mr^2} \frac{1}{\psi(r)} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi_n(r)}{\partial r} \right) + \frac{1}{Y} \frac{L^2 Y}{2mr^2} - \frac{e^2}{r} = E$$

$$\uparrow$$

$$L^2 Y = l(l+1) \hbar^2 Y$$

$$\rightarrow -\frac{\hbar^2}{2mr^2} \frac{1}{\psi(r)} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi_n(r)}{\partial r} \right) + \frac{\hbar^2 l(l+1)}{2mr^2} - \frac{e^2}{r} = E$$

$$\rightarrow -\frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi_n(r)}{\partial r} \right) + \left[ \frac{\hbar^2 l(l+1)}{2mr^2} - \frac{e^2}{r} \right] \psi_n(r) = E \psi_n(r)$$

~~A~~ A - continued

2

$$U = rR$$

$$\chi = r\psi \rightarrow \psi = \frac{\chi}{r}$$

$$\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \left[ \frac{\chi}{r} \right] = \frac{\partial}{\partial r} r^2 \left[ \frac{1}{r} \frac{d\chi}{dr} - \frac{\chi}{r^2} \right]$$

$$= \frac{\partial}{\partial r} \left[ r \frac{d\chi}{dr} - \chi \right]$$

$$= \cancel{\frac{d\chi}{dr}} + r \frac{d^2\chi}{dr^2} - \cancel{\frac{d\chi}{dr}}$$

$$\rightarrow -\frac{\hbar^2}{2m_1^2} r \frac{d^2\chi}{dr^2} + \left[ \frac{\hbar^2 \ell(\ell+1)}{2m_1^2} - \frac{e^2}{r} \right] \frac{\chi}{r} = E \frac{\chi}{r}$$

$$\rightarrow \boxed{-\frac{\hbar^2}{2m} \frac{d^2\chi}{dr^2} + \left[ \frac{\hbar^2 \ell(\ell+1)}{2m_1^2} - \frac{e^2}{r} \right] \chi = E \chi}$$

$\rightarrow$  remember  $m \rightarrow \mu$

Ⓒ Skip B  $\rightarrow$  I don't think you can do this without finishing the problem

$$\rightarrow r \rightarrow \infty \rightarrow \frac{d^2\chi}{dr^2} = -\frac{2mE}{\hbar^2} \chi$$

$\rightarrow$  For bound states  
 $E$  is -

$$\frac{d^2\chi}{dr^2} = \alpha^2 \chi$$

$$\text{where } \alpha = \sqrt{2mE}$$

$$\rightarrow \text{solution is } \chi_i = \cancel{e^{\alpha r}} e^{-\alpha r}$$

The  $e^{\alpha r}$  is not  
physically acceptable



(3)

(D)  $\chi_1(r) = f(r) e^{-\alpha r} = r e^{-\alpha r}$

lets not plug in  $f(r) = r$  yet

$$-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} [f(r) e^{-\alpha r}] + \left[ \frac{\hbar^2 \alpha^2}{2m} \right] f(r) e^{-\alpha r} = E f(r) e^{-\alpha r}$$

$$\frac{d}{dr} \left[ \frac{df}{dr} e^{-\alpha r} - \alpha f(r) e^{-\alpha r} \right]$$

$$\frac{d^2 f}{dr^2} e^{-\alpha r} - \frac{df}{dr} \alpha e^{-\alpha r} - \frac{df}{dr} \alpha e^{-\alpha r} + \alpha^2 f(r) e^{-\alpha r}$$

$$-\frac{\hbar^2}{2\mu} \left[ \frac{d^2 f}{dr^2} - \frac{df}{dr} \alpha - \frac{df}{dr} \alpha + \alpha^2 f(r) \right]$$

$\uparrow \quad \quad \uparrow \quad \quad \uparrow \quad \quad \uparrow$   
 $\emptyset \quad -\alpha \quad -\alpha \quad \alpha^2 r$

$$-2\alpha + \alpha^2 r = \alpha^2 r$$

assuming  
you make  
 $\alpha$  mistake  
and these

should cancel

$$E_1 = \frac{\alpha^2 \hbar^2}{2m}$$

(E)  $E_1 = \frac{\alpha^2 \hbar^2}{2m}$

$$E = K_g \frac{m^2}{s^2} = \alpha^2 K_g \frac{m^4}{s^2}$$

$$= \alpha^2 K_g \frac{m^4}{s^2}$$

$$K_g \frac{m^2}{s}$$

$$\alpha = \frac{1}{a_0}$$

F-2001

### Problem 6: Hydrogen Atom (10 Points)

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

$$\phi(r, \theta, \phi) = Ae^{-\left(\frac{r}{a_0}\right)}$$

where  $A$  and  $a_0$  (the Bohr radius) are constants.

- a) Find  $A$  by normalizing the wavefunction. Express your answer in terms of  $a_0$ . **(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)**

F-2008

①

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

$$\begin{aligned} \textcircled{A} \quad 1 &= \int_0^\infty \int_0^\pi \int_0^{2\pi} A^2 e^{-2r/a_0} r^2 \sin\theta \, d\phi \, d\theta \, dr = \int \phi \phi \\ &= 4\pi A^2 \int_0^\infty e^{-2r/a_0} r^2 \, dr \\ &= 4\pi A^2 \frac{\Gamma(2+1)}{(2/a_0)^{2+1}} = 4\pi A^2 \frac{2}{\left(\frac{2}{a_0}\right)^3} = 1 \\ &\rightarrow 8\pi A^2 \frac{a_0^3}{2^3} = 1 \rightarrow \boxed{A = \frac{1}{\sqrt{a_0^3}}} \end{aligned}$$

$$\textcircled{B} \quad V(r) = \cancel{\frac{e^2}{r}} \quad \text{Negative?}$$

$$\rightarrow \langle V \rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{1}{\cancel{4\pi a_0^3}} e^2 r e^{-2r/a_0} \sin\theta \, d\phi \, d\theta \, dr$$

$$\begin{aligned} \frac{2}{1/2} - \frac{1}{2} &= \frac{1}{2} \\ \frac{4}{2} - a &= \frac{3}{2} \\ &= a^{1/2} \end{aligned} \quad = \frac{4\pi e^2}{\cancel{4\pi a_0^3}} \int_0^\infty r e^{-2r/a_0} \, dr$$

$$\frac{\Gamma(1+1)}{(2/a_0)^{1+1}} = \frac{(1)a_0^2}{4}$$

$$= \frac{4\pi e^2 a_0^2}{\cancel{4\pi a_0^3}}$$

$$\boxed{\langle V \rangle = \frac{e^2}{a_0}}$$

$$\langle V \rangle = \frac{e^2}{a_0}$$

$$\begin{aligned}
 \textcircled{C} \langle r \rangle &= \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{1}{\frac{4\pi}{3} a_0^3} r^3 e^{-2r/a_0} \sin\theta d\phi d\theta dr \quad \textcircled{2} \\
 &= \frac{4\pi}{3 a_0^3} \int_0^\infty r^3 e^{-2r/a_0} dr \\
 &= \frac{\Gamma(3+1)}{\left(\frac{2}{a_0}\right)^{3+1}} = \frac{3! a_0^4}{2^4} \\
 &= \frac{6 a_0^4}{16} \\
 &= \frac{3 a_0^4}{8}
 \end{aligned}$$

$$\rightarrow \boxed{\frac{3}{2} a_0 = \langle r \rangle}$$

most probable  $\rightarrow P = \frac{1}{a_0^3} \int_0^\infty \int_0^\pi \int_0^{2\pi} r^2 e^{-2r/a_0} \sin\theta d\phi d\theta dr$

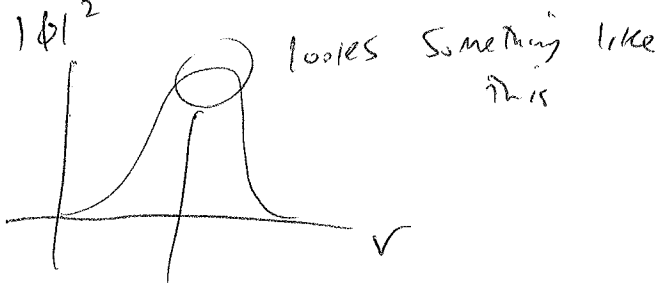
$$= \frac{4\pi}{a_0^3} \int_0^\infty r^2 e^{-2r/a_0} dr$$

$$\begin{aligned}
 \frac{dP}{dr} &= 0 = \frac{4}{a_0^3} \left[ \frac{e^{-2r/a_0}}{a} \left( r^3 - 2r^2 + \frac{2}{a} \right) + \frac{e^{-2r/a}}{a} \left( 2r - \frac{2}{a} \right) \right] \\
 &= \frac{4}{a_0^3} \left[ \frac{e^{-2r/a}}{a} \left( r^3 - 2r^2 + \frac{2}{a} \right) + \frac{e^{-2r/a}}{a} \left( 2r - \frac{2}{a} \right) \right]
 \end{aligned}$$

Most probable

(3)

Probability density distribution =  $|\phi|^2 = \frac{1}{a_0^3} r^2 e^{-2r/a_0} \sin^2 \theta$



This is the most probable

$$\rightarrow \frac{dP}{dr} = 0 = \frac{d}{dr} \left[ \frac{1}{a_0^3} r^2 e^{-2r/a_0} \sin^2 \theta \right]$$

$$= \frac{\sin^2 \theta}{a_0^3} \left[ 2r e^{-2r/a_0} - \frac{2r^2}{a_0} e^{-2r/a_0} \right]$$

$$= 0$$

$$1 - \frac{r}{a_0} = 0$$

$$1 - \frac{r}{a_0} = 0$$

$$\boxed{r = a_0}$$

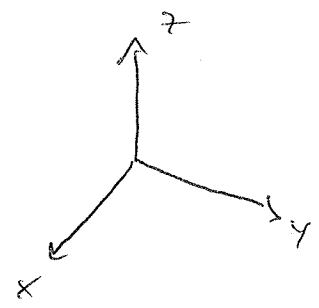
(4)

(D)  $\langle L \rangle = \int \phi^* L \phi d^3r$

$\uparrow$   
 All space      real

$$= \int L \phi^2 d^3r$$

$$\begin{aligned} \rightarrow L &= r \times p \\ &= r p \sin\theta \\ &= -i\hbar \nabla \sin\theta \end{aligned}$$



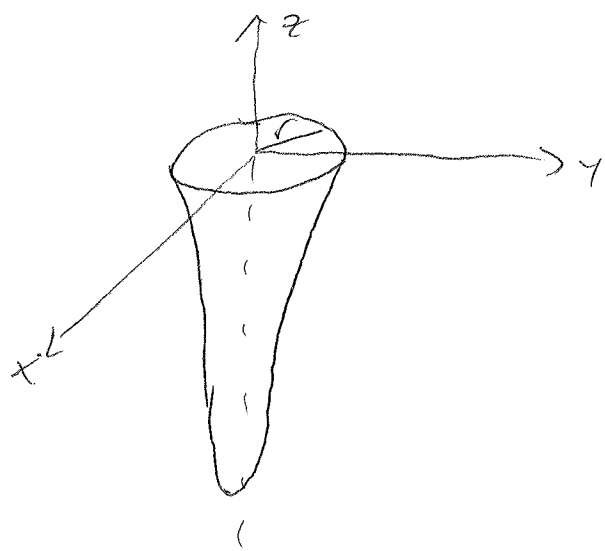
without doing the integral, the answer will be imaginary. Since the ~~approx~~ expectation value is observable,

$\langle L \rangle = 0$

compared to the Bohr model where

$\langle L \rangle = \hbar$

(e)



The potential is Spherically Symmetric in the xy plane

$z$  corresponds to the direction of the measurable angular momentum in the  $z$  direction

$$L_z = \hbar \sin\theta$$