Discussion 13

Quick exercises

1. State the value of the ground state energy of hydrogen.
2. From the above, compute the Rydberg constant, which is the (inverse) wavelength of a photon with energy E_1. State the result in inverse nanometers.
3. An excited hydrogen atom emits an ultraviolet photon, and relaxes into a lower energy state. Which orbital is the electron in afterwards?
4. In the special case where ℓ is maximum ($\ell = n - 1$) the radial wavefunctions has only one bump. Show that this causes the radial probability density $r^2|R|^2$ to have a bump at location $r_{peak} = n^2 a_0$, where a_0 is the Bohr radius.

Problems

5. At time $t = 0$ a hydrogen atom is in the state

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2}}|1,0,0\rangle + \frac{1}{\sqrt{2}}|2,1,1\rangle$$

where $|n, \ell, m\rangle$ are the simultaneous energy, total angular momentum, and orbital angular momentum eigenstates of the hydrogen atom.

   (a) What is the state at a later time, t?
   (b) Compute the expectation value of the energy.
   (c) Compute the expectation value of the total angular momentum, $\langle L^2 \rangle$.
   (d) Compute the expectation value of the z component of the angular momentum, $\langle L_z \rangle$.
   (e) Compute $\langle L_x \rangle$ and $\langle L_y \rangle$ (Hint: use $L_x = \frac{1}{2}(L_+ + L_-)$ and $L_y = \frac{1}{2i}(L_+ - L_-)$).

6. List the degeneracies of the first 3 energy levels of hydrogen, neglecting the existence of spin. What is the pattern? Confirm the pattern by counting the degeneracy of the *nth* level.

7. (a) Find $\langle r \rangle$ and $\langle r^2 \rangle$ for an electron in the ground state of hydrogen. Express your answer in terms of the Bohr radius.
   (b) Find $\langle x \rangle$ and $\langle x^2 \rangle$ in the ground state of hydrogen. Hint: No new integration required. Remember that $r^2 = x^2 + y^2 + z^2$, and the ground state is spherically symmetric.
   (c) Find $\langle x^2 \rangle$ in the state $n = 2$, $\ell = 1$, $m = 1$. Note that this state does *not* have spherical symmetry.

Discussion 10 solutions

1 $E_1 = \dfrac{-\alpha^2 m_e c^2}{2} = \boxed{-13.6\,\text{eV}}$

2 $R_\infty = \dfrac{|E_1|}{hc} = \dfrac{13.6\,\text{eV}}{1240\,\text{eV}\cdot\text{nm}} = \boxed{0.0109\ \text{nm}^{-1}}$

3 Only transitions to the 1s state are energetic enough to create UV photons
$\Rightarrow$ final state is 1s.

4 For $l = n-1$, the radial wavefunction is proportional to

$$R_{n,l}(r) \propto r^l e^{-r/na}$$

up to normalization. We want to find the maximum of $r^2|R_{nl}(r)|^2$, which is the same as maximizing $r R_{nl}(r)$:

$$\frac{d}{dr}\left(r^{l+1} e^{-r/na}\right) = 0$$

$$\Rightarrow \quad n r^{n-1} e^{-r/na} - \frac{1}{na} r^n e^{-r/na} = 0$$

$$\Rightarrow \quad n r^{n-1} = \frac{1}{na} r^n$$

$$\Rightarrow \quad n = \frac{1}{na} r_{peak}$$

$$\Rightarrow \quad \boxed{r_{peak} = n^2 a}$$

5

(a) $\boxed{|\Psi(t)\rangle = \frac{1}{\sqrt{2}} e^{-iE_1 t/\hbar} |1,0,0\rangle + \frac{1}{\sqrt{2}} e^{-iE_2 t/\hbar} |2,1,1\rangle}$

where $E_n = -\frac{1}{2}\alpha^2 m_e c^2$.

(b) $\langle E\rangle = \frac{1}{2}\cdot E_1 + \frac{1}{2}\cdot E_2 = \boxed{-\frac{5}{8}\left(\frac{\alpha^2 m_e c^2}{2}\right)}$

(c) $\langle L^2\rangle = \frac{1}{2}\cdot 0 + \frac{1}{2}\cdot 2\hbar^2 = \boxed{\hbar^2}$

(d) $\langle L_z\rangle = \frac{1}{2}\cdot 0 + \frac{1}{2}\cdot \hbar = \boxed{\hbar/2}$

(e) Use $L_x = \frac{1}{2}(L_+ + L_-)$, so

$$\langle L_x \rangle = \langle \Psi | L_x | \Psi \rangle = \frac{1}{2} \langle \Psi | (L_+ + L_-) | \Psi \rangle .$$

Need only compute at $t=0$ since $\langle L_x \rangle$ is conserved.

$$L_+ |\Psi\rangle = \frac{1}{\sqrt{2}} \underbrace{L_+ |1,0,0\rangle}_{0} + \frac{1}{\sqrt{2}} \underbrace{L_+ |2,1,1\rangle}_{0} = 0$$

$$L_- |\Psi\rangle = \frac{1}{\sqrt{2}} \underbrace{L_- |1,0,0\rangle}_{0} + \frac{1}{\sqrt{2}} \underbrace{L_- |2,1,1\rangle}_{\sqrt{2}\hbar |2,1,0\rangle} = \hbar |2,1,0\rangle$$

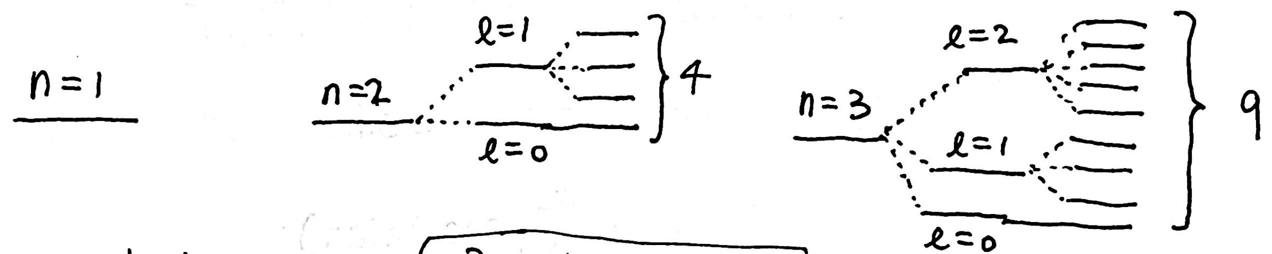
Then:

$$\langle L_x \rangle = \left(\frac{1}{\sqrt{2}} \langle 1,0,0| + \frac{1}{\sqrt{2}} \langle 2,1,1| \right) \left(\hbar |2,1,0\rangle \right) = \boxed{0}$$

Because they're orthogonal $\langle n, \ell, m | n', \ell', m' \rangle = 0$ unless $n=n'$, $\ell = \ell'$, $m = m'$.

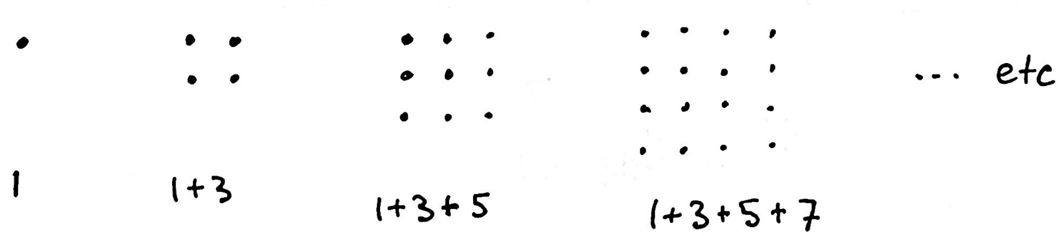
(f) Similarly, $\langle L_y \rangle = \frac{1}{2i} \langle \Psi | (L_+ - L_-) | \Psi \rangle = \boxed{0}$.

$\boxed{6}$



Pattern looks like $\boxed{n^2 \text{ degeneracy.}}$

Can confirm: the sum of the first n odd numbers is n^2



$\boxed{7}$ The ground state of hydrogen is:

$$\Psi_{100}(r,\theta,\varphi) = 2a^{-3/2}\, e^{-r/a} \left(\underbrace{\frac{1}{\sqrt{4\pi}}}_{Y_{00}} \right)$$

(a) $$\langle r \rangle = 4a^{-3} \int_0^\infty dr\, r^3 e^{-2r/a} = 4a^{-3} \cdot \frac{3}{8} a^4 = \boxed{\frac{3}{2} a}$$

$$\langle r^2 \rangle = 4a^{-3} \int_0^\infty dr\, r^4 e^{-2r/a} = 4a^{-3} \cdot \frac{3}{4} a^5 = \boxed{3a^2}$$

(b) The state is symmetric about $x=0$ so $\boxed{\langle x \rangle = 0}$

Next, because $r^2 = x^2 + y^2 + z^2$ and because of spherical symmetry $\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle$ so

$$\boxed{\langle x^2 \rangle = \frac{1}{3} \langle r^2 \rangle = a^2}$$

(c) Use $$R_{21}(r) = \frac{1}{2\sqrt{6}}\, a^{-3/2} \left(\frac{r}{a}\right) e^{-r/2a}$$

$$Y_{11}(\theta,\varphi) = -\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta\, e^{i\varphi}$$

We want $\langle x^2 \rangle$, where $x = r\sin\theta\cos\varphi$. This is given by:

$$\langle x^2 \rangle = \iiint dV\, (r\sin\theta\cos\varphi)^2\, |\Psi_{211}|^2$$

$$= \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta\, \sin\theta \int_0^\infty dr\, r^2\, (r\sin\theta\cos\varphi)^2\, \frac{1}{24a^5} \left(\frac{3}{8\pi}\right) \sin^2\theta\, r^2 e^{-r/a}$$

Have:

$$\int_0^{2\pi} d\varphi\, \cos^2\varphi = \pi \qquad \int_0^{\pi} d\theta\, \sin^5\theta = \frac{16}{15} \qquad \int_0^\infty dr\, r^6 e^{-r/a} = 720a^7$$

$$\Rightarrow \langle x^2 \rangle = \frac{1}{24a^5}\left(\frac{3}{8\pi}\right) \cdot \pi \cdot \frac{16}{15} \cdot 720a^7 = \boxed{12a^2}$$