Homework 8

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A One-Dimensional Atom

1. The probability of finding an electron in a range may be found using $P = \int_a^b |\psi(x)|^2 \, dx$

$$P = \int_0^{a_o} |\psi(x)|^2 \, dx$$

$$\psi(x) = 2x \left(\frac{1}{a_o}\right)^{\frac{3}{2}} e^{-\frac{x}{a_o}}$$

$$\int_0^{a_o} \frac{4x^2}{a_o^3} e^{-\frac{2x}{a_o}} \, dx$$

$$\frac{4}{a_o^3} \int_0^{a_o} x^2 e^{-\frac{2x}{a_o}} \, dx$$

Using a mathematical solver, we get:

$$\frac{4}{a_o^3} \int_0^{a_o} x^2 e^{-\frac{2x}{a_o}} \, dx = .323$$

There is a 32.3% probability the electron is in this range

Hydrogen Atom Wave Functions

2. The possible quantum numbers are:

n	l	m_l	m_s
4	0	0	$\pm 1/2$
4	1	-1	$\pm 1/2$
4	1	0	$\pm 1/2$
4	1	1	$\pm 1/2$
4	2	-2	$\pm 1/2$
4	2	-1	$\pm 1/2$
4	2	0	$\pm 1/2$
4	2	1	$\pm 1/2$
4	2	2	$\pm 1/2$
4	3	-3	$\pm 1/2$
4	3	-2	$\pm 1/2$
4	3	-1	$\pm 1/2$
4	3	0	$\pm 1/2$
4	3	1	$\pm 1/2$
4	3	2	$\pm 1/2$
4	3	3	$\pm 1/2$

Hydrogen Atom Wave Functions 2

3. We know the spherical wave equation is:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial\Psi}{\partial r}+\frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial\Psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right]+U(r)\Psi(r,\theta.\phi)=E\Psi(r,\theta,\phi)$$

We also know that the ground state wave function of a hydrogen atom is:

$$\psi=\frac{1}{\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{\frac{3}{2}}e^{-\frac{r}{a_o}}$$

$$\frac{2}{r}\frac{\partial\Psi}{\partial r}=-\frac{2}{r\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{\frac{5}{2}}e^{-\frac{r}{a_o}}$$

$$\frac{\partial\Psi^2}{\partial r^2}=\frac{1}{\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{\frac{7}{2}}e^{-\frac{r}{a_o}}$$

Plugging this into the differential equation, we get:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{\frac{7}{2}}e^{-\frac{r}{a_o}}-\frac{2}{r\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{\frac{5}{2}}e^{-\frac{r}{a_o}}\right]+U(r)\Psi=E\Psi$$

This can be rewritten as:

$$-\frac{\hbar^2}{2m}\left[\left(\frac{1}{a_o}\right)^2\cancel{\Psi}-\frac{2}{ra_o}\cancel{\Psi}\right]+U(r)\cancel{\Psi}=E\cancel{\Psi}$$

We know E is independent of r, so we get:

$$E=-\frac{\hbar^2}{2m}\left(\frac{1}{a_o}\right)^2$$

Because we know that $a_o=\frac{4\pi\varepsilon_o\hbar^2}{me^2}$, we can plug this in:

$$E=-\frac{\hbar^2}{2m}\frac{m^2e^4}{\hbar^4}=-\frac{me^4}{32\pi^2\varepsilon_o^2\hbar^2}$$

This means $E_o=-13.6[\text{eV}]$; thus, this is a valid solution.

Radical Probability Densities

4. The radial wave function of the state where $n = 2$ and $l = 0$ is:

$$\psi = \left(2 - \frac{r}{a_o}\right)\left(\frac{1}{a_o}\right)^{\frac{3}{2}} e^{-\dfrac{r}{2a_o}}$$

The probability density is given by:

$$P_{2,0} = 4\pi r^2 |\psi|^2$$

Differentiating this and setting it equal to 0 will yield the highest probability value:

$$\frac{d}{dr}\left(4\pi r^2 |\psi|^2\right) = 0$$

This becomes:

$$\frac{d}{dr}\left(4\pi r^2 \left(2 - \frac{r}{a_o}\right)^2 \left(\frac{1}{a_o}\right)^3 e^{-\frac{r}{a_o}}\right)$$

Simplifying, this turns into:

$$\frac{d}{dr}\left(\left(\frac{16\pi r^2}{a_o^3} - \frac{16\pi r^3}{a_o^4} + \frac{4\pi r^4}{a_o^5}\right) e^{-\frac{r}{a_o}}\right)$$

Differentiating, this becomes:

$$\left(\frac{32\pi r}{a_o^3} - \frac{48\pi r^2}{a_o^4} + \frac{16\pi r^3}{a_o^5}\right) e^{-\frac{r}{a_o}} - \frac{1}{a_o}\left(\frac{16\pi r^2}{a_o^3} - \frac{16\pi r^3}{a_o^4} + \frac{4\pi r^4}{a_o^5}\right) e^{-\frac{r}{a_o}} = 0$$

The exponential terms cancel out, which leaves us with:

$$\left(\frac{32\pi r}{a_o^3} - \frac{64\pi r^2}{a_o^4} + \frac{32\pi r^3}{a_o^5} - \frac{4\pi r^4}{a_o^6}\right) = 0$$

Simplifying further:

$$8 - \frac{16r}{a_o} + \frac{8r^2}{a_o^2} - \frac{r^3}{a_o^3} = 0$$

Using a numerical solver, the roots of this are found to be:

$$r = 2a_o, (3 \pm \sqrt{5})a_o$$

Peaks occur at $r = (3 \pm \sqrt{5})a_o$

Intrinsic Spin

5. (a) The degeneracy may be calculated using the formula $2n^2$; for the $n = 5$ energy level, it is found that there are $2n^2 = 2(5)^2 = 50$ degeneracies

   (b) The possible combinations for $n = 5$ are as follows:

$$n = 5 l = \begin{cases} 0, & m_l = 0 \\ 1, & m_l = \begin{cases} 0 \\ \pm 1 \end{cases} \\ 2, & m_l = \begin{cases} 0 \\ \pm 1 \\ \pm 2 \end{cases} \\ 3, & m_l = \begin{cases} 0 \\ \pm 1 \\ \pm 2 \\ \pm 3 \end{cases} \\ 4, & m_l = \begin{cases} 0 \\ \pm 1 \\ \pm 2 \\ \pm 3 \\ \pm 4 \end{cases} \end{cases}$$

Counting the possible values, there are 25. When including spin in the calculation, this doubles the degeneracy values, as, for any quantum number, spin may be $\pm\frac{1}{2}$. As such, there are $2(25) = 50$ degeneracies