Modern Physics II - HW6 Solution - Winter 2016

1. Derive and calculate the Bohr radius and ground state energy for deuterium from the second order ordinary differential equation that describes radial dependencies within the Schrödinger model of the hydrogen atom. Hints: you need a wavefunction, you have to use the concept of reduced mass of the electron. State your results with numbers and their proper physical SI units for full credit (5 points)

Beginning with the radial equation:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2\mu}{\hbar^2}\left[E-V-\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}\right]R=0$$

Ground state so we can set ℓ to zero:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2\mu}{\hbar^2}\left[E-V\right]R=0$$

Using the product rule to sort out the left term a bit:

$$\frac{1}{r^2}\left[2r\frac{dR}{dr}+r^2\frac{d^2R}{dr^2}\right]+\frac{2\mu}{\hbar^2}\left[E-V\right]R=0$$

$$\frac{2}{r}\frac{dR}{dr}+\frac{d^2R}{dr^2}+\frac{2\mu}{\hbar^2}\left[E-V\right]R=0$$

Plugging in the electrostatic potential:

$$\frac{2}{r}\frac{dR}{dr}+\frac{d^2R}{dr^2}+\frac{2\mu}{\hbar^2}\left[E+\frac{e^2}{4\pi\varepsilon_0 r}\right]R=0$$

Now we can use a general solution for R, don't worry too much about rationalizing the form, it's possible derive with a bit unit analysis and is an exponential by inspection of the previous equation. The general solution for other states though is a bit more involved and requires associated Laguerre polynomials, but we get to avoid that for now since ℓ is zero:

$R = Ae^{-r/a_0}$, normalization constant A, and a_0 with units length.

Using this as a solution:

$$\frac{2}{r}\left(-\frac{1}{a_0}Ae^{-r/a_0}\right)+\left(\frac{1}{a_0{}^2}Ae^{-r/a_0}\right)+\frac{2\mu}{\hbar^2}\left[E+\frac{e^2}{4\pi\varepsilon_0 r}\right]\left(Ae^{-r/a_0}\right)=0$$

$$\left(-\frac{2}{ra_0}+\frac{1}{a_0{}^2}+\frac{2\mu}{\hbar^2}\left[E+\frac{e^2}{4\pi\varepsilon_0 r}\right]\right)\left(Ae^{-r/a_0}\right)=0$$

$$-\frac{2}{ra_0}+\frac{1}{a_0{}^2}+\frac{2\mu}{\hbar^2}E+\frac{2\mu e^2}{4\pi\varepsilon_0 r\hbar^2}=0$$

Paring up the terms with the same units:

$$\left(\frac{1}{a_0{}^2}+\frac{2\mu}{\hbar^2}E\right)+\left(\frac{2\mu e^2}{4\pi\varepsilon_0\hbar^2}-\frac{2}{a_0}\right)\frac{1}{r}=0$$

So noting we need to have both of these terms equal to zero, we can split the equation up and use our length term to help us get the energy:

$$\frac{2\mu e^2}{4\pi\varepsilon_0\hbar^2}-\frac{2}{a_0}=0$$

$$\frac{2}{a_0}=\frac{2\mu e^2}{4\pi\varepsilon_0\hbar^2}$$

$$a_0=\frac{4\pi\varepsilon_0\hbar^2}{\mu e^2}$$

This gives us an expression for the most likely radius the electron is from the nucleus, or Bohr's radius. Using this result we can solve for the energy as well:

$$\frac{1}{a_0{}^2}+\frac{2\mu}{\hbar^2}E=0$$

$$E=-\frac{\hbar^2}{a_0{}^2 2\mu}$$

$$=-\left(\frac{\mu e^2}{4\pi\varepsilon_0\hbar^2}\right)^2\frac{\hbar^2}{2\mu}$$

$$=-\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2$$

Which should be comforting since this matches up with the Bohr energy levels as well.

Taking our results and plugging in reduced mass:

$$\mu = \frac{m_d m_e}{m_d + m_e} \approx \frac{2m_p m_e}{2m_p + m_e} \approx \frac{2\left(1.673\text{E-}27_{kg}\right)\left(9.109\text{E-}31_{kg}\right)}{2\left(1.673\text{E-}27_{kg}\right)+\left(9.109\text{E-}31_{kg}\right)} \approx 9.107\text{E-}31_{kg}$$

$$\begin{aligned} a_0 &= \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2} \\ &\approx 52.93_{pm} \end{aligned}$$

$$\begin{aligned} E &= -\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \\ &\approx -2.179\text{E-}18_J \\ &\approx -13.60_{eV} \end{aligned}$$

Which pretty much looks like normal hydrogen (as it should) if we took a few more sig figs we would see that there is a slight deviation which what causes the slight spectral shift between hydrogen and deuterium.

2. Calculate the expectation value of r for the radial part of the wavefunction for the ground state of the hydrogen atom. 3 points if your numerical value is correct and given with its proper SI unit. Why does your result differ from the Bohr radius? 2 points

Fairly strait forward, starting with the normalized wavefunction for the radial component of the ground state:

$$\Psi = \frac{2}{a_0^{3/2}} e^{-r/a_0}$$

Need to get the expectation so in the usual way:

$$\begin{aligned} \langle r \rangle &= \int \Psi^* r \Psi dr \\ &= \frac{4}{a_0^3}\int_0^\infty r^3 e^{-2r/a_0} dr \quad \text{, spherical integration and now by parts} \\ &= \frac{4}{a_0^3}\left[-\frac{a_0}{2} r^3 e^{-2r/a_0}\Big|_0^\infty - \int_0^\infty \left(-3r^2 \frac{a_0}{2} e^{-2r/a_0} \right) dr \right] \text{, and by parts again, chaining out} \\ &= \frac{4}{a_0^3}\left[\left(-\frac{a_0}{2} r^3 - 3\left(\frac{a_0}{2}\right)^2 r^2 - 6\left(\frac{a_0}{2}\right)^3 r - 6\left(\frac{a_0}{2}\right)^4 \right) e^{-2r/a_0} \right]_0^\infty \\ &= \frac{4}{a_0^3}\left[0+0+0+6\left(\frac{a_0}{2}\right)^4 \right] \\ &= \frac{3}{2} a_0 \end{aligned}$$

Taking this result we can plug in the Bohr radius for a_0:

$$\langle r \rangle = \frac{3}{2}a_0 \approx \frac{3}{2}\left(52.9_{pm}\right) \approx 79.3_{pm}$$

Of course the answer differs from the Bohr radius because this is the average location of the electron, not the most probable location. Purely from an argument of symmetry the only way you could have the average at the same location as the central peak is if the distribution was equally weighted about that peak. Just eyeballing the distribution though we can see that there is more "probability area" to the right of the peak so we should assume that the average would also be to the right of the peak.

3. The Dirac theory of the hydrogen atom delivers $\sqrt{3/4}\hbar$ *for the magnitude of the spin angular momentum vector. Naively assuming that an electron were a tiny sphere (of 5x10*$^{-17}$ *m) that would be spinning about its own axis, calculate how fast it would need to be spinning, i.e. the tangential instantaneous velocity on its surface perpendicular to the axis. 6 points. How does your result compare to the speed of light in a vacuum? 1 point. What can you conclude about the spin of an electron from your calculation and comparison? 2 points and 1 more point if all physical units are correct in your calculations and answer.*

Assuming a tiny uniformly dense ball with radius $5\text{E-}17_m$ of with the mass of an electron with an angular momentum of $\sqrt{3/4}\hbar$ we can lean against a classical solution to figure out how fast this thing is rotating.

Starting with angular momentum:

$$L = I\omega$$

Next we know that the moment of inertia for a rotating sphere is:

$$I = \frac{2}{5}mr^2$$

Plugging in the mass of an electron and the radius given results in:

$$I \approx 9.109\text{E-}64_{kg\cdot m^2}$$

A particularly tiny number but no worries. We were given L so all we need to do is use that to solve for ω.

$$\omega = \frac{L}{I} \approx \frac{\sqrt{3/4}\left(1.055\text{E-}34_{kg\cdot m^2/s}\right)}{9.109\text{E-}64_{kg\cdot m^2}} \approx 1.003\text{E}29_{rad/s}$$

Using that result we can figure out what the tangential velocity is on the edge of the sphere furthest from the rotating axis is:

$$V_{\tan} = r\omega \approx (1.003\text{E}29_{rad/s})(5\text{E-}17_{m}) \approx 5.013\text{E}12_{m/s}$$

This of course is an unfortunately unrealistic answer. Comparing to the speed of light:

$$\frac{V_{\tan}}{c} \approx \frac{5.013\text{E}12_{m/s}}{3.00\text{E}8_{m/s}} \approx 1.67\text{E}4$$

Which is considerably faster than the speed of light, implying there is a serious problem with thinking about an electron as a tiny spinning ball (the classical interpretation). Since the electrons dimensions have an upper bound placed on them due to scattering experiments we can't just scale up the size to take care of the problem, so it would appear that there is no classical model solution for representing electron spin.