EP Homework 9

Adam Kit - 3707437

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1 Average Distance

The wave function in equation 1 describes a particle in a potential field.

$$\Psi(r) = Ae^{\frac{-r^2}{2a_0^2}} \tag{1}$$

For an operator or value x the corresponding expectation value can be found to be:

$$\langle x \rangle = \int \bar{\Psi}(x) x \Psi(x) dx \tag{2}$$

In 2 $\bar{\Psi}(x)$ represents the complex conjugate of $\Psi(x)$.

We must find the average distance of the particle from the center of the potential field, which can be found using the spherical coordinate equation below:

$$\langle r \rangle = \int_0^\infty \Psi r \Psi 4\pi r^2 dr$$

Plugging in our Ψ we see:

$$\langle r \rangle = \int_0^\infty Ae^{\frac{-r^2}{2a_0^2}} rAe^{\frac{-r^2}{2a_0^2}} 4\pi r^2 dr = 4\pi A^2 \int_0^\infty r^3 e^{\frac{-r^2}{a_0^2}} dr$$

Using U-substitution, with $u = -r^2$ we have:

$$= 4\pi A^2 \int_0^\infty \frac{1}{2} e^{\frac{u}{a_0^2}} u du$$

Then integration by parts: $p = u$, $v' = e^{\frac{u}{a_0^2}}$

$$= 4\pi A^2 \frac{1}{2} \left(a_0^2 e^{\frac{u}{a_0^2}} u - \int a_0^2 e^{\frac{u}{a_0^2}} du \right) = 4\pi A^2 \frac{1}{2} \left(a_0^2 e^{\frac{u}{a_0^2}} u - a_0^4 e^{\frac{u}{a_0^2}} \right) = 4\pi A^2 \frac{1}{2} \left(a_0^2 e^{\frac{-r^2}{a_0^2}} (-r^2) - a_0^4 e^{\frac{-r^2}{a_0^2}} \right)$$

$$= 2\pi A^2 a_0^2 e^{\frac{-r^2}{a_0^2}} \left(-r^2 - a_0^2 \right)$$

Then we fill in the boundry conditions of $r = 0$ and $r = \infty$

$$= (0 - 2\pi A^2 a_0^2(-a_0^2)) = 2\pi A^2 a_0^4 = \langle r \rangle$$

This is visualized in Figure 1 and the code for the rest of the figures can be found in this repository.

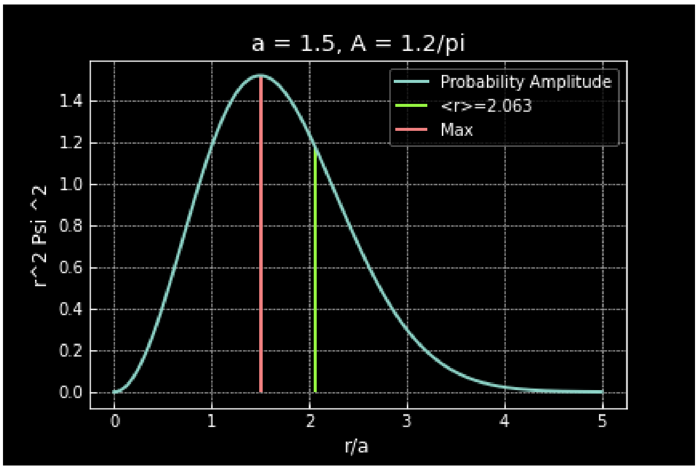

Figure 1: The probability amplitude for a wave function described by $\Psi(r) = Ae^{-r^2/2a0^2}$. The average distance $\langle r \rangle$ from the potential field is plotted (green) as well as the position of maximum probability (pink). One may note that the units are incorrect, but that is becasuse we are technically looking at dimensionless quantity for a and A, so this is only to aid in visualization and is not supposed to represent with accuracy a hydrogen-like atom.

2 Inverse Distance

For a hydrogen atom with quantum numbers $n = 1$, $l = 0$, the radial wave function is given in the lecture notes (Eq. 1.258) as 3.

$$R_{1,0}(r) = 2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-\frac{Zr}{a_0}} \tag{3}$$

So for the hydrogen atom, $Z = 1$ and 3 becomes:

$$R_{1,0} = \frac{2}{a_0^{\frac{3}{2}}} e^{-r/a_0}$$

And the inverse expected distance is:

$$\langle r^{-1} \rangle = \int_0^\infty \Phi_{1s} r^{-1} \Phi_{1s} 4\pi r^2 = 1$$

For the Hydrogen Atom in the ground state, $n = 1$, we see that the maximum value of the probability amplitude corresponds to the inverse distance $\langle r^{-1} \rangle$ as seen in figure 2. For the case where $n = 2$, we have a radial wave function of:

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

Which will have an inverse expected distance $\langle r^{-1} \rangle$ of $6/a_0$. A visualization aid is found in Figure 3.

3 Average Energy

For the ground state of the Hydrogen Atom we have the quantum numbers $n = 1$, $l = 0$, thus the same wave function as in 3, but with the angular included: $Y_{1,0} = \frac{1}{\sqrt{4\pi}}$. Using our relationship 2, we find the

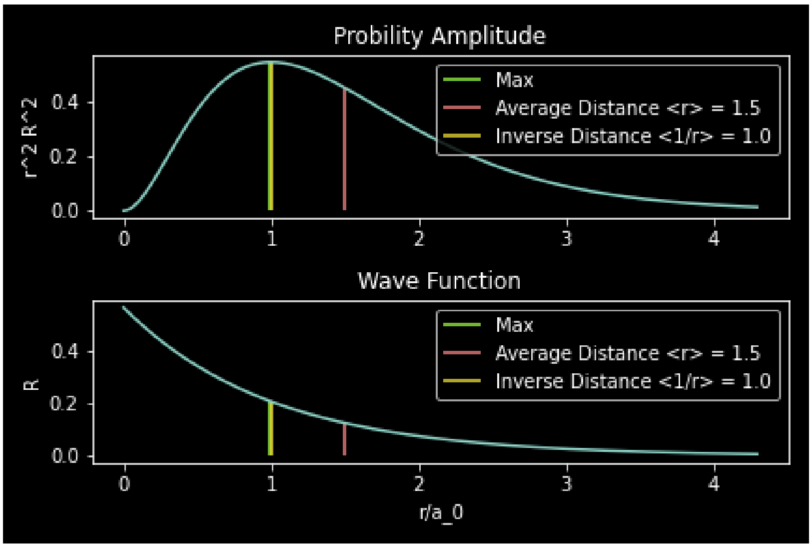

Figure 2: The probability amplitude for the ground state hydrogen atom $n = 1, l = 0$. The average distance $\langle r \rangle$from the potential field is plotted (pink) as well as the inverse $\langle r^{-1} \rangle$ (gold). As seen in the graph, the inverse corresponds to the maximum. $a_0 = 1$

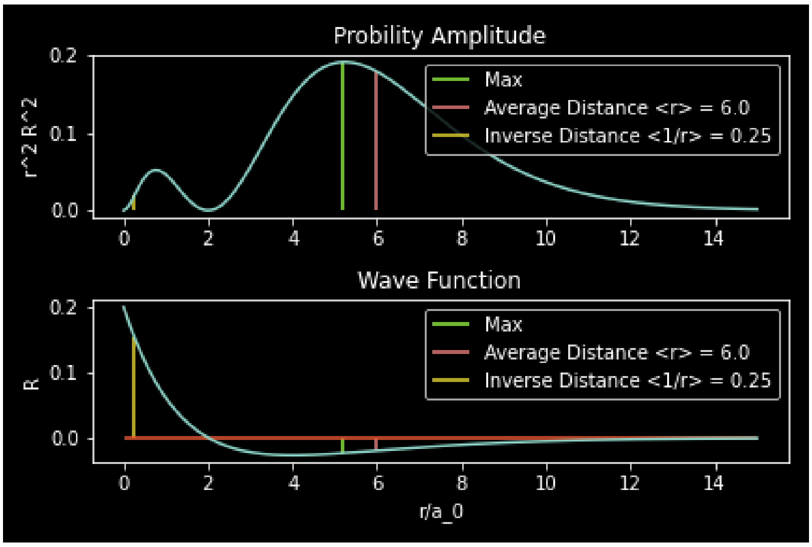

Figure 3: The probability amplitude and wave function for the hydrogen atom with quantum numbers $n = 2, l = 0$. The average distance $\langle r \rangle$from the potential field is plotted (pink), the maximum probability (green), as well as the inverse $\langle r^{-1} \rangle$ (gold). Here the inverse distance is not equal to the maximum! $a_0 = 1$

kinetic energy to be:

$$\langle T\rangle = \int_0^\infty \Psi(r)\left(-\frac{\hbar^2}{2m}\Delta\Psi(r)\right)4r^2dr = \int_0^\infty \Psi(r)\frac{\hbar}{2m}\left(\frac{2}{a^{3/2}}\right)\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}e^{-r/a_0}\right]4r^2dr$$

$$= \int_0^\infty \Psi(r)\frac{\hbar}{2m}\left(\frac{2}{a^{3/2}}\right)\left[-\frac{2}{ra_0}e^{-r/a_0}+\frac{1}{a_0^2}e^{-r/a_0}\right]4r^2dr = \frac{-\hbar^2}{2m}\frac{4}{a_0^3}\int_0^\infty\left(-\frac{2r}{a_0}e^{-2r/a_0}+\frac{r^2}{a_0^2}e^{-2r/a_0}\right)dr$$

$$= -\frac{\hbar^2}{2m}\frac{4}{a_0^3}\left(\frac{-a_0}{4}\right) = \frac{\hbar^2}{2ma_0^2}$$

The potential energy is found similarly, but instead of the laplace operation, we use the inverse distance like problem 2, since the potential has the relationship $-\frac{e^2}{r}$.

$$\langle V\rangle = \int_0^\infty \Psi(r)\left(-\frac{e^2}{r}\right)\Psi(r)4\pi r^2 = -\frac{4e^2}{a_0^3}\int_0^\infty re^{-2r/a_0}dr = -\frac{e^2}{a_0}$$

One can validate the relationship

$$e^2 = \frac{\hbar^2}{ma_0} \Rightarrow \langle V\rangle = -\frac{\hbar^2}{ma_0^2}$$

3.1 Virial Theorem

We can now check the Virial Thm.

$$\langle T\rangle = -\frac{1}{2}\langle V\rangle$$

. Which obviously holds. The average total energy is then

$$\langle E\rangle = \langle T\rangle + \langle V\rangle = -\frac{\hbar^2}{2ma_0^2} = -13.6eV$$

This is exactly our energy for the ground state electron of the Hydrogen atom.

4 Angular Momentum

For an electron in the d-state, $l = 2$, and the angular momentum can be found from the relationship in the lecture notes (eq 1.236):

$$L^2 = l(l+1)\hbar^2 \Rightarrow L = \sqrt{l(l+1)}\hbar^2$$

So the angular momentum for this electron would be $L = \sqrt{2(3)}\hbar = \sqrt{6}\hbar$. For the Z-component, one sees that

$$\hat{L}_z\Psi = -i\hbar\frac{\partial}{\partial\phi}(R(r)Y(\phi,\vartheta)) = -i\hbar\frac{\partial}{\partial\phi}\left(R(r)\Theta(\vartheta)\Phi(\phi)\right) = -i\hbar R(r)\Theta(\vartheta)\frac{\partial}{\partial\phi}e^{im\phi} = m\hbar\Psi$$

$$\Rightarrow \langle L_z\rangle = m\hbar$$

Interesting to note that since $l^2 > m^2$, we can see that $L^2 > L_z^2$. Also, the maximal projection onto any axis is limited by l, i.e, only a maximum of l units can be measured along any given direction, as seen in figure 4.

References

[1] Nave, Carl
http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/vecmod.html

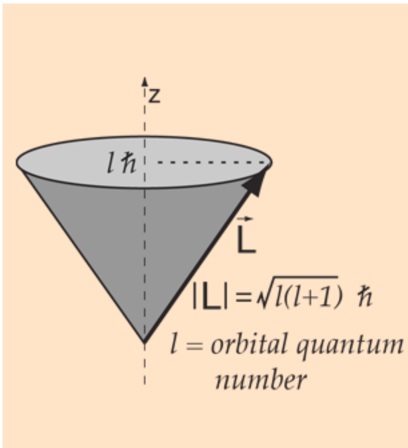

Figure 4: Orbital Angular Momentum for an atomic electron visualized.[1]