

Chem 30324, Spring 2018, Homework 4

Due February 21, 2018

In a “1-dimensional hydrogen atom”, an electron is confined to the positive x axis and attracted to a proton at the origin. The potential felt by the electron can be written as

$$V(x) = \begin{cases} -C\frac{1}{x} & \text{if } x > 0 \\ \infty & \text{if } x \leq 0 \end{cases}$$

where $c = \frac{e^2}{4\pi\epsilon_0} = \frac{\hbar^2}{m_e a_0}$ is a bunch of constants with units energy times distance.

In particular, m_e is the electron mass and a_0 is the bohr radius, a convenient unit of length equal to 0.529 Å. It's easiest to solve the problems below using the second set of constants. Further, the following equations are often of use in solving problems related to this system:

$$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}, \quad \frac{d}{dx} x e^{-ax} = e^{-ax}(1 - ax), \quad \frac{d^2}{dx^2} x e^{-ax} = a e^{-ax}(ax - 2)$$

1. Write down the time-independent Schrödinger equation for the 1-D H atom. Remember to include the domain of the equation.

2. Would $\phi(x) = e^{ikx}$ be an acceptable wavefunction for this system? Why or why not?

3. Consider the candidate wavefunction $\psi_1(x) = \frac{x}{a_0} e^{-x/a_0}$. Plot $V(x)$ and $\psi_1(x)$. Be sure to label axes appropriately. (Hint: it is convenient to work in units of a_0 . That is, make your plots against x/a_0 .)

4. Is $\psi_1(x)$ normalized? If not, construct the normalized $\tilde{\psi}_1(x)$. It is ok to express your answer in terms of fundamental constants.

5. What is the most probable distance of the electron from the proton, in units of a_0 ?

6. What is the probability of finding the electron further than a_0 from the proton?

7. If you measure the linear momentum of many electrons, all with the same wavefunction $\tilde{\psi}_1(x)$, will you get the same answer every time? What will you get on average? It is ok to express your answer in terms of fundamental constants.

8. If you measure the total energies of many electrons, all with the same wavefunction $\tilde{\psi}_1(x)$, will you get the same answer every time? What will you get on average? (*Hint*: It will help to express $V(x)$ in terms of a_0 , \hbar , and m_e .)

9. The normalized wavefunction $\tilde{\psi}_2(x) = \frac{x}{\sqrt{2}a_0^{3/2}}(1 - \frac{x}{2a_0})e^{-x/2a_0}$ is an eigenfunction of the one-dimensional H atom Schrödinger equation with eigenvalue $E_2 = -\frac{\hbar^2}{8m_e a_0^2}$. Plot $\tilde{\psi}_2(x)$. Are $\tilde{\psi}_1(x)$ and $\tilde{\psi}_2(x)$ orthogonal? (Be sure to justify your answer!)

10. Suppose an electron is in a superposition state described by $\xi(x) = \frac{1}{\sqrt{3}}(\tilde{\psi}_1(x) + \sqrt{2}\tilde{\psi}_2(x))$. If you measure the total energies of many electrons, all with the same wavefunction $\xi(x)$, will you get the same answer every time? What will you get on average? It is ok to express your answer in terms of fundamental constants.

11. The uncertainties in the positions of an electron described by $\tilde{\psi}_1(x)$ and $\tilde{\psi}_2(x)$ can be shown to be $2^{1/2}a_0$ and $6^{1/2}a_0$, respectively. Contrast the uncertainties in their linear speeds.