The Hydrogen Atom in Wave Mechanics

Michael Brodskiy
Professor: Q. Yan

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1 A One-Dimensional Atom

- Analyzing a Hydrogen Atom in Quantum Mechanics
  - The potential energy, derived from the Coulomb force, is:

$$U(r) = -\frac{e^2}{4\pi\varepsilon_o r}$$

  - This may be converted to be in terms of x, and plugged into the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - \frac{e^2}{4\pi\varepsilon_o x}\psi(x) = E\psi(x)$$

  - To keep this finite, the following two conditions need to be met:

$$\begin{cases} x \to 0, & \psi(x) = 0 \\ x \to \infty, & \psi(x) = 0 \end{cases}$$

  - Using $\psi(x) = Axe^{-bx}$ with the Schrödinger equation, solving would obtain:

$$\boxed{b = \frac{me^2}{4\pi\varepsilon_o\hbar^2} = \frac{1}{\alpha_o} \Rightarrow \text{Bohr Radius}}$$

  - Using the normalization condition, and $\psi(x) = Axe^{-bx} = Axe^{\frac{x}{\alpha_o}}$, we get:

$$A = \frac{2}{\alpha_o^{\frac{3}{2}}}$$

  - Conclusions:
    * For the ground state, there is an uncertainty in the location of e^-
    * The most probable region to find e^- is near $x = \alpha_o$ (consistent with Bohr model)
    * But, it's possible to find e^- anywhere (which is very difference from Bohr)

2 Angular Momentum in the Hydrogen Atom

  - The angular momentum in a planetary system is constant, and vector $\vec{L}(L_x, L_y, L_z)$ has three components
    * l is the angular momentum quantum number; it determines the length of the vector
    * m_l is the magnetic number; it determines one of the components of the vector

* We have:

$$|\vec{L}| = \sqrt{l(l+1)}\hbar, \qquad l = 0, 1, 2\cdots$$

$$\vec{L}_z = m_l\hbar, \qquad m_l = 0, \pm1, \pm2, \cdots \pm l$$

* We know l and m_l for $\vec{L}_z$, but what is the direction?
* Applying the uncertainty principle, we obtain:

$$\Delta\vec{L}_z\Delta\phi \geq \hbar$$

3 The Hydrogen Atom Wave Functions

- Moving from a unidimensional case to a tridimensional case, we try to apply the Schrödinger equation (in Cartesian coordinates):

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + U(x,y,z)\psi(x,y,z) = E\psi(x,y,z)$$

- The potential energy is:

$$U(x,y,z) = -\frac{e^2}{4\pi\varepsilon_o}\frac{1}{\sqrt{x^2+y^2+z^2}}$$

- The wave function may be defined as:

$$\psi(x,y,z) = X(x)Y(y)Z(z)$$

- Converting to polar coordinates to make calculations simpler, the Schrödinger equation becomes:

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

- The wave function then becomes

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$$

  - Where R is the radial function, Θ is the polar function, and Φ is the azimuthal function
  - This breaks ψ into 3 equations, making the wave function easier to solve for

- The defined quantum numbers are as follows:

Number	Name	Values
n	Principle	$1, 2, 3, \cdots$
l	Angular Momentum	$0, 1, 2, \cdots, n-1$
m_l	Magnetic	$0, \pm 1, \pm 2, \cdots, \pm l$