29/05/2020

Atomic structure and Quantum mechanics.

Time independent schrodinger wave equation:

$$\left[\frac{-h^2}{8\pi^2 m}\bar{\nabla}^2 + E_p(x, y, z)\right]\psi(x, y, z) = E\,\psi(x, y, z)$$

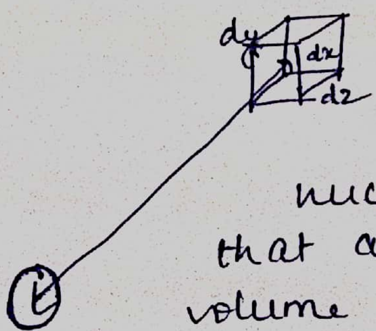
$$\boxed{\hat{H}\psi = E\psi} \text{ ——— } (1)$$

The solution of this equation for stationary state potential energy which is analogous to the stationary state or stading-wave equations for vibrating springs gives the posible values of ψ functions.

These ψ functions having a posible solution is called eigenfunctions or wave functions.

The solution of these functions gives the value of corresponding energies called eigenvalues.

Eigenfunctions and normalizations:



The volume elements dx dy dz are at the distance r from the nucleus. The probability that an election is in the volume element is proportional to the $\psi^2\,dx\,dy\,dz$ if ψ is real and $\psi\psi^*dx\,dy\,dz$ when ψ is complex.

If the value of ψ is normalized, the probability is equal to $\psi\psi^*\,dx\,dy\,dz$.

- The eigenfunctions provide the information about the probability density of an election.

The eigenfunctions must justify some of the basic conditions:-

→ They must be single valued.

→ finite in all regions in space.

→ They must be continuous.

why???

→ i) For the first condition to be single valued it must be clear that probability in any region can have only one value.

→ ii) for the finite part, schrodinger equation will not apply to the electron where ψ is infinite and hence the electron does not acts as wave.

→ iii) discontinuties are not possible in nature.

Overall the eigen function must be square integral.

$$\int \psi^2(x, y, z)\, dx\, dy\, dz$$

over all time and space.

→ eigen function however may be complex that is, it contain $i = \sqrt{-1}$.

→ complex function can carry both real and imaginary part and is written as $(a + ib)$ whose square is $(a^2 - b^2 + 2iab)$ which is also imaginary and hence can not represent a probability

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→ To avoid such difficulty complex conjugate ψ^* is added and probability is given by $\psi\psi^*$ where ψ^* is $(a-ib)$ and hence the product is a^2+b^2 which is real.

Normalization:

If we multiply ψ by any number 'a', we get

$$\hat{H}(a\psi) = E(a\psi)$$

and probability of electron in the space $dx\,dy\,dz$ is

$$(\psi\psi^*\,dx\,dy\,dz)$$

On integration of this over all space

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi\psi^*\,dx\,dy\,dz = 1$$

can be written as $\boxed{\int\psi\psi^*\,d\tau = 1}$

$d\tau = dx\,dy\,dz$ ⇒ normalized condition

Hence the equation becomes:-

$$\int\phi\phi^*\,d\tau = b$$

where ϕ is the eigen function obtained after the solution of Schrodinger wave equation

To make the equation an integral unity:

$$\int\frac{\phi\phi^*}{\sqrt{b}\sqrt{b}}\,d\tau = 1$$

The new function becomes $\psi = \phi\sqrt{b}$

The equation

$$\int\psi\psi^*\,d\tau = 1 \text{ is}$$

known as normalized condition.

Postulates in quantum mechanics:

Postulate I: The physical state of particle is described fully as possible by an appropriate wave function $\psi(x, y, z, t)$

Postulate II: The possible wave functions $\psi(x, y, z, t)$ are obtained by solving the Schrodinger wave equation.

$$\left[\frac{-h^2}{8\pi^2 m}\nabla^2 + E_p(x, y, z)\right]\psi = E\psi$$

by keeping boundary conditions into account.

Postulate III: Every dynamical variable, corresponding to the physically observable property can be represented by linear operator. i.e. $\hat{O}(a\psi + b\phi) = a\hat{O}\psi + b\hat{O}\phi$

Two operators can commute :- $\hat{O}_1\hat{O}_2\psi = \hat{O}_2\hat{O}_1\psi$

Question:-

If operator x is one dimensional position operator and $\left(\frac{h}{2\pi i}\right)\frac{\partial}{\partial x}$ is one dimensional momentum operator. Prove that they commute!

→ class at 6:00 p.m today evening. →

Keep studying

Stay Home and stay safe:

kindly go through both the sheets I shared before the class