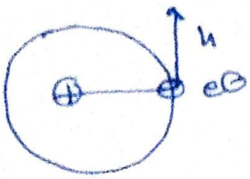
Quantum mechanics

Bohr equation of energy in Hydrogen and hydrogen like



$$Ze^2/r^2 = mu^2/r$$

centripetal   centrifugal

$$u^2 = \frac{Ze^2}{r^2} \cdot \frac{r}{m} = \frac{Ze^2}{mr} \quad \text{— ①}$$

Acc. to Bohr postulates $mur = \frac{nh}{2\pi}$ (Angular momentum)

$$u = \frac{nh}{2\pi mr} \quad \text{— ②}$$

or $$u^2 = \left(\frac{n^2h^2}{4\pi^2m^2r^2}\right) \quad \text{— ③}$$

now from ① and ③ we have

$$\frac{Ze^2}{\cancel{m}r} = \frac{n^2h^2}{4\pi^2m^{\cancel{2}}r^{\cancel{2}}}$$

$$Ze^2 = \frac{h^2n^2}{4\pi^2mr}$$

$$\therefore \quad r \equiv r_n = \frac{n^2h^2}{4\pi^2Ze^2m}$$

for hydrogen atom $n=1$

$$r_1 = a_0 = \frac{h^2}{4\pi^2me^2}$$

Total energy is given by sum of KE and PE

$$E = \frac{1}{2}mu^2 - \frac{Ze^2}{r_n}$$

$$mu^2 = \frac{Ze^2}{r_n} \quad \text{(from eqn 1)}$$

also $$E = \frac{1}{2}\frac{Ze^2}{r_n} - \frac{Ze^2}{r_n} = \frac{-Ze^2}{2r_n}$$

$$E = \frac{-Ze^2}{2} \times \frac{4\pi^2 Zme^2}{n^2h^2}$$

$$\boxed{E_n = -\frac{2\pi^2 Z^2 me^4}{n^2h^2}}$$

Bohr's effect

SI

$$r_n = \frac{(4\pi\epsilon_0) n^2h^2}{4\pi^2 Zme^2}$$

$$E_n = \frac{-2\pi^2 Z^2 me^4}{(4\pi\epsilon_0)^2 n^2h^2}$$

$4\pi\epsilon_0$ is called permittivity factor and its value is $1.11264 \times 10^{-10}\ C^2N^{-1}m^{-2}$.

$$a_0 = r_1 = \frac{(4\pi\epsilon_0)h^2}{4\pi^2me^2} = 0.529 \times 10^{-10}\ m$$

Velocity of electron:

$$v_1 = \frac{nh}{2\pi mr} = 2.188 \times 10^6\ ms^{-1}$$

$$E_2 = \frac{-2\pi^2me^4}{(4\pi\epsilon_0)^2 n_2^2h^2} \quad \text{and } E_1 = \frac{-2\pi^2me^4}{(4\pi\epsilon_0)^2 n_1^2h^2}$$

$$\Delta E = h\nu = \frac{2\pi^2 me^4}{(4\pi\epsilon_0)^2 h^2}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$\bar{\nu} = \frac{1}{\lambda} = \frac{\nu}{c} = \frac{2\pi^2me^4}{(4\pi\epsilon_0)^2h^3c}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$= R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

R_H - Rydberg's constant

$= 109690.8\ cm^{-1}$

$= 29.79 \times 10^{-19}\ J$

$= 13.6\ eV$

n_1 lyman

n_2 Balmer

n_3 Paschen

n_4 Brackett

n_5 Pfund

Sommerfeld's extension of Bohr's Theory:

$$\frac{n}{k} = \frac{\text{length of major axis}}{\text{length of minor axis}}$$

n= principal quantum number

k= azimuthal quantum number.

Acc. to this theory energy of an e- does not only depend upon principal quantum number but on azimuthal quantum number too.

Heisenberg Uncertainity Principle:

It is imposible to simultaneously detemine the exact position and velocity of a minute moving particle like an e⁻.

wave particle duality of electron:

Einstein in 1905 suggested that light has dual nature as wave as well as particle.

Louis de Broglie also proposed that matter has dual character as wave as well as particle.

$$\boxed{\lambda = \frac{h}{mu}}$$ de Broglie eqn.

also $E = mc^2$

since $h\nu = mc^2$

$$\nu = \frac{c}{\lambda}$$

$$\frac{hc}{\lambda} = mc^2$$

$$\frac{h}{\lambda} = mc$$

$$\lambda = \frac{h}{mc} = \frac{h}{p}$$ $p = mc$ = linear momentum

Distinction b/w matter wave and electromagnetic wave:

matter waves are different from e/m bcos:

→ speed is very less

→ These waves can't be radiated in empty spaces.

→ They are not emitted by particle under consideration but associated c̄ it.

→ λ value very small.

Derivation of Bohr Angular momentum from de Broglies

$$\lambda = \frac{h}{mv}$$

$$2\pi r = n\lambda$$

$$\frac{nh}{mv} = 2\pi r$$

$$L = mvr$$

$$L = \frac{nh}{2\pi}$$

* If the circumference is bigger or smaller than $\frac{nh}{2\pi}$ the wave will no longer remain in phase.

Heisenberg Uncertainity Principle:

It is not possible to determine the position and momentum of small moving particle.

$$(\Delta x)(\Delta p_x) \geq \frac{h}{4\pi}$$

Compton effect:

Compton found that on falling on carbon or some other light element, the scattered X-rays have λ larger than incident rays. In other words the scattered xrays have lower frequency or energy than incident x-rays. Since scattering is caused by electron it is proved that there is some interaction b/w e- and X-rays. This ↓se in E or ↑se in λ is called compton effect

Relation between classical mechanics and quantum mechanics

$v <<< c$ (velocity of macroscopic bodies is far less than the velocity of light c, relativistic mechanics gives the same result as ~~quantum~~ mechanics of Newton.

for $h \to 0$, the time dependent schrodinger eqn changes to Newton's second law.

Postulates of quantum mechanics:

i) The physical state of a system is defined by the time is given as wavefunction $\psi(x,t)$.

ii) The wavefuncn $\psi(x,t)$ and its first and second derivative $\partial\psi(x,t)/\partial x$ and $\partial^2\psi(x,t)/\partial x^2$ are continuous finite and single valued for all values of x. $\psi(x,t)$ is normalized. i.e.

~~iii)~~
$$\int_{-\infty}^{\infty} \psi^*(x,t)\,\psi(x,t)\,dx = 1$$

ψ^* complex conjugate of ψ formed by replacing i to $-i$ wherever it occurs in the function ψ ($i = \sqrt{-1}$)

III) A physically observable quantity can be represented by a Hermitian operator. An operator $\hat{A}$ is said to be Hermitian if it satisfies the following condition.

$$\int \psi_i^* \hat{A} \psi_j \, dx = \int \psi_j (\hat{A}\psi_i)^* dx$$

ψ_i and ψ_j are wavefunctions representing the physical states of quantum system, such as particle, an atom or a molecule.

iv) The allowed values of an observable A are the eigen values a_i in the operator eqn.

$$\hat{A}\psi_i = a_i\psi_i \quad \text{— eigenvalue eqn}$$

v) The average value of $\langle A \rangle$ of an observable A corresponding to operator $\hat{A}$ is obtained from the relation

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi \, dx$$

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* \hat{x} \psi \, dx$$

vi) The quantum mechanical operators corresponding to the observables are constructed by writing the classical expressions in terms of variables

classical variable	quantum mechanical operator	operator	operation
x	$\hat{x}$	x	
p_x	$\hat{p}_x$	$-i\hbar \frac{\partial}{\partial x}$	
x^2	$\hat{x}^2$	x^2	
p_x^2	$\hat{p}_x^2$	$-h^2 \frac{\partial^2}{\partial x^2}$	
t	$\hat{t}$	t	
E	$\hat{E}$	$i\hbar \frac{\partial}{\partial t}$	