Difference Between classical and quantum Mechanics.

(i) classical Mechanics.

- classical mechanics viewed energy transfer as continuous. For example
- " when you drop an object from a height The potential energy it had at the height it continuously transferred to "K.E" as it falls and gain speed."
- classical mechanics deals with the motion of objects under forces of Their own momentum
- classical mechanics describes The motion of macroscopic object such as spacecrafts planets, and galaxies.

(ii) Quantum Mechanics.

Quantum mechanics deals with microscopic object. It is much more complicated. but it provides accurate results for particles of even very small size.

Quantum mechanics handles the wave-particle dulity of atom and molecules.

- Quantum mechanics views energy transferred as quantized. For example
- The object at the height is an energy state and when you drop it that's energy is given off all at once and moves to a lower energy state.
- It deal the behaviour of objects at the microscopic level.

Drive quantum Number for Hydrogen atom.

Quantum Number

Application of schrodinger wave equation for hydrogen atom tells us that only certain energy levels are allowed. The wave function "ψ" and the probability, ψ^2 unable to us calculate the region in space where the electron is most likely found. These region are called "atomic orbital. The allowed orbital are determine by a set of number is called "quantum Numbers. These quantum are determines the energy of a particlar orbitals and spaced accupied by the orbital. In order to describe an e^-

in an atom four quantum number are required.

Principal Quantum Number. "n"

This quantum numbers denotss the principal—shell to which the electron belong. It represent the energy and averge size of the electron cloud. As electron with $n=1$ has lowest energy and is bound most firmly to the nucleous.

Energy level or shells also be designated by the latter K, L, M, N, O, P and Q

Principal quantum number "n"	= 1	2	3	4
	= K	L	M	N
Maximum Number of alatron $= 2n^2 =$	2	8	18	32

Azimuthal quantum Number (l)

It define the spatial distribution of the electron cloud about the nucleous. It define the shape of the orbitals accupied by the electron. The value of 'l' depend upon the 'n'. For a given value of 'n'. The azimuthal quantum l can have all integral values from 0 to $n-1$ each of which refers to amergy sublevel. Each shell a subshell equal to principal quantum Number. The sub-shell depend upon the value of azimuthal quantum number

$(l = n-1)$

Magnetic quantum Number.

This quantum are purposed to account for the spliting up of spectral lines in an atomic spectrum under the influence of strong magnetic field. mi give information about the orientation of an orbital in space. so It is also called orientation quantum number. The possible value of mi depend upon 'l'. The value of mi will be (2l+1). when l=0 than m=0

for l=1, the mi will have three values +1, 0, -1 which mean three orientation for p orbital px, py, and pz depend upon axis of orientation.

Derivation of Magnetic quantum Number.

The Φ equation generally written as

$$\frac{1}{\Phi} \cdot \frac{d^2\Phi}{d\phi^2} = -m^2 \quad \text{---} (1)$$

$$\frac{d^2\Phi}{d\phi^2} = -\phi m^2$$

$$\frac{d^2\phi}{d\phi^2} + \phi m^2 = 0 \quad \text{---} (2)$$

It is second order differential equation. So, above equation (2) can be written as

$$\phi = A \sin m\phi + B \cos m\phi$$

One of the requirment for such function is that it is must be sin refer to met this restriction.

The function ϕ should have the same value it has for $\phi = 2\pi$ since these are identical angular position. otherwise the value of ϕ at the same position will lead to two different way

$\psi = R\,\Theta\,\phi$ and hance two different values of $\psi\psi^*$

for the case $\phi = 0$

$$\phi(0) = A\sin(0) + B\cos(0) = B$$

when $\phi = 2\phi$

$$\phi(2\phi) = [A\sin(2\pi) + B\cos(2\pi)]m$$

As value of ϕ same under both these condition.

$$B = A\sin m(2\pi) + B\cos m(2\pi)$$

" Represent the constant by " m^2 "

$$-\frac{1}{\phi}\frac{d^2\phi}{d\phi^2} = m^2 \quad - (2.102)$$

equation (2.102) is called ϕ equation which on solution gives the magnitude of let

$$\frac{\sin^2\theta}{R_r}\cdot\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\cdot R_r\right)+\frac{\sin\theta}{\Theta_\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{\partial}{\partial\theta}\Theta_\theta\right)-m^2+$$

$$\frac{8\pi^2 m}{h^2}\cdot r^2\sin^2\theta\left(\frac{ze^2}{r}+E\right)=0$$

Dividing eq. above with " $\sin^2\theta$ "

$$\frac{1}{R_r}\cdot\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\cdot R_r\right)+\frac{1}{\sin\theta\,\Theta_\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{\partial}{\partial\theta}\Theta_\theta\right)-$$

$$-\frac{m^2}{\sin^2\theta}+\frac{8\pi^2 m}{h^2}\cdot r^2\left(\frac{ze^2}{r}+E\right)=0$$

Combining 1st + 4th part and 2nd + 3rd

$$\frac{1}{R_r}\cdot\frac{\partial}{\partial r}\left(\frac{r^2\partial}{\partial r}R_r\right)+\frac{8\pi^2 m}{h^2}\cdot r^2\left(\frac{ze^2}{r}+E\right)=\text{“}\beta\text{”}$$

Solution for ϕ

let

$$-\frac{1}{\phi}\frac{d^2\phi}{d\phi^2}=m \quad - \quad (2.102)$$

equation (2.102) is called ϕ equation which on solution gives The magnitude of of magnetic quantum Number. So L.H.S of eq (2.102) also equal to "m^2"

$$\frac{\sin^2\theta}{r}\cdot\frac{d}{dr}\left(r^2\cdot\frac{dR}{dr}\right)+\frac{\sin\theta}{\theta}\cdot\frac{d}{d\theta}\left(\sin\theta\cdot\frac{d\theta}{d\theta}\right)+\frac{8\pi^2\mu}{h^2}\left(E+\frac{Ze^2}{4\pi\varepsilon_0 r}\right)r^2\cdot\sin^2\theta=m^2$$

So, above equation contain two variable but they may be separate by dividing the equation by $\sin^2\theta$.

on re-arranging we get

$$\frac{1}{R}\cdot\frac{d}{dr}\left(r^2\cdot\frac{dR}{dr}\right)+\frac{8\pi^2\mu}{h^2}\left(E+\frac{Ze^2}{4\pi\varepsilon_0 r}\right)r^2=\frac{m^2}{\sin^2\theta}$$

$$-\frac{1}{\theta\sin\theta\, d\theta}\left(\sin\theta\cdot\frac{d\theta}{d\theta}\right)$$

Each side of above equation has one variable and because the equation hold for all variable value of r and θ. Each side of the equation must have constant value which representing this constant by "β"

$$\frac{1}{R}\cdot\frac{d}{dr}\left(r^2\cdot\frac{dR}{dr}\right)+\frac{8\pi^2\mu}{h^2}\left(E+\frac{Ze^2}{4\pi\varepsilon_0 r}\right)r=\beta \quad (2.103)$$

Multiplying eq (2.103) by R/r^2 we get

$$\frac{1}{r^2}\cdot\frac{d}{dr}\left(r^2\cdot\frac{dR}{dr}\right)+\frac{8\pi^2\mu}{h^2}\left(E+\frac{Ze^2}{4\pi\varepsilon_0 r}\right)R=\frac{\beta R}{r^2}$$

$$\frac{1}{r^2}\cdot\frac{d}{dr}\left(r^2\cdot\frac{dR}{dr}\right)+\frac{8\pi^2\mu}{h^2}\left(E+\frac{Ze^2}{4\pi\varepsilon_0 r}\right)R-\frac{\beta R}{r^2}=0 \quad (2.104)$$

eq (2.104) eq is called R- equation. on solution it give principal quantum number (n)

Similarly equation R. Has also 'β'

$$\frac{m^2}{\sin^2\Theta}-\frac{1}{\Theta\sin\Theta\, d\Theta}\cdot\frac{d}{d\Theta}\left(\sin\Theta\cdot\frac{d\Theta}{d\Theta}\right)=\beta$$

Multiplying Θ and re-arranging eq.

$$-\frac{1}{\sin\Theta}\cdot\frac{d}{d\Theta}\left(\sin\Theta\cdot\frac{d\Theta}{d\Theta}\right)=\beta\Theta-\frac{m^2\Theta}{\sin^2\theta}$$

$$\frac{1}{\sin\theta}\cdot\frac{d}{d\Theta}\left(\sin\theta\cdot\frac{d\Theta}{d\Theta}\right)+\left(\beta\Theta-\frac{m^2}{\sin^2\theta}\right)\Theta=0$$

Derivation of principal quantum number. "n"

In The Hydrogen atom, where The electron density has spherical symmetry, all The derivatives depending on the angular properties θ and ϕ will disapear. The Simplification eq (31) to the form.

$$\frac{1}{r^2} \cdot \frac{\partial}{\partial r}\left(r^2 \cdot \frac{\partial \psi}{\partial r}\right) + \frac{8\pi^2 m}{h^2}\left(E + \frac{e^2}{r}\right)\psi = 0$$

$$\frac{\partial^2}{\partial r^2}\psi + \frac{2}{r} \cdot \frac{\partial \psi}{\partial r} + \frac{8\pi^2 m}{h^2}\left(E + \frac{e^2}{r}\right)\psi = 0$$

A spherical solution will have the form

$$\psi = e^{-ra}$$

$$\frac{\partial \psi}{\partial r} = -a \cdot e^{-ra}$$

oR

$$\frac{\partial^2 \psi}{\partial r^2} = a^2 \cdot e^{-ra}$$

Putting the value of $\frac{\partial^2 \psi}{\partial r^2}$ into eq. we get,

$$a^2 \cdot e^{-ra} + 2r(-a \cdot e^{-ra}) + \frac{8\pi^2 m}{h^2}\left(E + \frac{e^2}{r}\right) e^{-ra} = 0$$

$$e^{-ra}\left[a^2 - \frac{2a}{r} + \frac{8\pi^2 m}{h^2}\left(E + \frac{e^2}{r}\right)\right] = 0$$

Since $e^{-ra} \neq 0$ for all value of 'r'

$$a^2 - \frac{2a}{r} + \frac{8\pi^2 m}{h^2}\left(E + \frac{e^2}{r}\right) = 0 \quad - (35)$$

when 'r' is very Large then $\frac{-2a}{r}$ and $\frac{e^2}{r}$ become very small, so above eq becomes.

$$a^2 + \frac{8\pi^2 m}{h^2} E = 0$$

OR

$$E = -\frac{a^2 h^2}{8\pi^2 m} \quad - (36)$$

substituting the value of 'E' from eq (36) into eq. (35), we have

$a^2 = \frac{16\pi^4 m^2 e^2}{h^4}$, so, substituting the value of (a^2) into eq. (36)

$$E = -\frac{2\pi^2 m e^4}{h^2} \quad \text{OR} \quad \boxed{E = -\frac{2\pi^2 m e^4}{h^2 n^2}}$$

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The Radial equation (Angular ..)

The form of radial equation has been known Since long before the advent of quantum mechanics The solution of 'R' to this equation satisfy the boundary condition. It turns out that the ground State wave function of Hydrogen atom is characterized by quantum Numbers $l = 0$ $m_l = 0$, So The radial equation is simple.

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu}{h^2}\left[E - V(r)\right]R = 0$$

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \frac{2\mu}{h^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)R = 0$$

So, The solution is taken as $R = A e^{-r/\varepsilon_0}$ ∴ A is normalization constant and a_0 is a length with electron ground state. So

$$\frac{dR}{dr} = -\frac{1}{a_0}R \text{ and } \frac{d^2R}{dr^2} = R/a_0^2$$

$$\left(\frac{1}{a_0^2} + \frac{2\mu E}{h^2}\right) + \frac{1}{r}\left(\frac{2\mu e^2}{4\pi\varepsilon_0 h^2} - 2/a_0\right) = 0$$

So, The only one way eq holds for all "r" if each term is equal to zero.

$$a_0 = \frac{4\pi\varepsilon_0 h^2}{\mu e^2}$$

$$E = -\frac{h^2}{2\mu a_0^2} = -E_0 \text{, we have.}$$

$$\frac{1}{\sin\theta}\cdot\frac{\partial}{\partial\theta}\sin\theta\frac{\partial\Theta}{\partial\theta} + \left(\lambda - \frac{m^2}{\sin^2\theta}\right)\Theta = 0$$ (angular Part)