Unit 4

Quantum Mechanics

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* Schrodinger time dependent wave equation

Consider a particle of mass 'm' is travelling along x-axis with a speed of 'V'. Then its wave function can be expressed as;

$$\boxed{\Psi(x,t) = Ae^{i(k_x x - \omega t)}} \quad \text{--- (1)}$$

where,

$$P_x = \hbar k_x$$

$$\text{or, } \boxed{k_x = \frac{P_x}{\hbar}} \quad \text{--- (2)}$$

and

$$E = \hbar\omega$$

$$\text{or, } \boxed{\omega = \frac{E}{\hbar}} \quad \text{--- (3)}$$

Using eq^n (2) and (3) in eq^n (1) we get,

$$\Psi(x,t) = Ae^{i\left(\frac{P_x}{\hbar} \times x - \frac{E}{\hbar} \times t\right)} \quad \text{--- (4)}$$

Differentiating eq^n (4) partially w.r.t. x we get,

$$\frac{\partial \Psi(x,t)}{\partial x} = Ae^{i(P_x/\hbar \times x - E/\hbar \times t)} \times \left(\frac{iP_x}{\hbar}\right)$$

$$\text{or, } \frac{\partial \Psi(x,t)}{\partial x} = \cancel{Ae}\left(\frac{iP_x}{\hbar}\right) \times \Psi(x,t)$$

Again differentiating ~~eq^n~~ partially w.r.t. x we get,

$$\frac{\partial}{\partial x}\left(\frac{\partial \psi(x,t)}{\partial x}\right) = \left(\frac{i p_x}{\hbar}\right) \frac{\partial \psi(x,t)}{\partial x}$$

or, $$\frac{\partial^2 \psi(x,t)}{\partial x^2} = \left(\frac{i p_x}{\hbar}\right) \times \left(\frac{i p_x}{\hbar}\right) \cdot A e^{i(p_x/\hbar \times x - E/\hbar \times t)}$$ [using eqⁿ ⑤]

or, $$\frac{\partial^2 \psi(x,t)}{\partial x^2} = \frac{-p_x^2}{\hbar^2} \psi(x,t)$$ (using eqⁿ ④)

or, $$\frac{\hbar^2 \partial^2 \psi(x,t)}{\partial x^2} = -p_x^2 \psi(x,t)$$

Dividing both sides by '2m'

$$\frac{\hbar^2 \partial^2 \psi(x,t)}{2m\, \partial x^2} = \frac{-p_x^2 \psi(x,t)}{2m}$$

or, $$\boxed{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} = \frac{p_x^2}{2m} \cdot \psi(x,t)}$$ —— ⑥

Again, differentiating eqⁿ ④ partially w.r.t. 't' we get,

$$\frac{\partial \psi(x,t)}{\partial t} = A e^{i(p_x/\hbar \times x - E/\hbar \times t)} \times \left(-\frac{iE}{\hbar}\right)$$

or, $$\frac{\partial \psi(x,t)}{\partial t} = \psi(x,t) \times \left(-\frac{iE}{\hbar}\right)$$ (using eqⁿ ④)

or, $$\frac{\hbar}{-i} \frac{\partial \psi(x,t)}{\partial t} = E \psi(x,t)$$

or, $$\frac{\hbar \times i}{-i \times i} \frac{\partial \psi(x,t)}{\partial t} = E \cdot \psi(x,t)$$

or, $$\boxed{i\hbar \frac{\partial \psi(x,t)}{\partial t} = E \psi(x,t)}$$ —— ⑦ $[\because i^2 = -1]$

For non-relativistic particle,

$$E = KE + P.E$$

$$E = \frac{P_x^2}{2m} + V_x$$

or, $$E\psi(x,t) = \frac{P_x^2}{2m}\psi(x,t) + V_x\,\psi(x,t)$$

Using eqⁿ ⑥ and ⑦ we get,

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V_x\,\psi(x,t)$$

or, $$\boxed{i\hbar\frac{\partial\psi(x,t)}{\partial t} = \left(\frac{-\hbar^2\partial^2}{2m\,\partial x^2} + V_x\right)\psi(x,t)}$$

This is 1-dimensional schrodinger's time wave dependent equation.

In 3-D,

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} = \left[\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V_r\right]\psi(r,t)$$

or, $$\boxed{i\hbar\frac{\partial\psi(r,t)}{\partial t} = \left[\frac{-\hbar^2}{2m}\nabla^2 + V_{(r)}\right]\psi(r,t)}$$

where,

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\therefore \boxed{i\hbar\frac{\partial\psi(r,t)}{\partial t} = \hat{H}\psi(r,t)}$$

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where,

$$\hat{H} = \frac{-\hbar^2 \nabla^2}{2m} + V_r$$

= Hamiltanian operator

Schrodinger's Time Independent Wave Equation

Consider a particle of mass 'm' is travelling along x-axis with a speed of 'v'. Then, its wave function can be expressed as,

$$\Psi(x,t) = Ae^{i(k_x x - \omega t)} \quad \text{--- (I)}$$

where,

$$P_x = \hbar k_x$$

$$\text{or, } k_x = \frac{P_x}{\hbar} \quad \text{--- (II)}$$

And,

$$E = \hbar\omega$$

$$\text{or, } \omega = \frac{E}{\hbar} \quad \text{--- (III)}$$

Now, using eqn (II) and (III) in eqn (I) we get,

$$\Psi(x,t) = Ae^{i\left(\frac{P_x}{\hbar} \times x - \frac{E}{\hbar} \times t\right)} \quad \text{--- (IV)}$$

Differentiating eqn (IV) partially w.r.t x, we get,

$$\frac{d\Psi(x,t)}{dx} = Ae^{i(P_x/\hbar \times x - E/\hbar \times t)} \times \left(\frac{iP_x}{\hbar}\right)$$

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or, $\frac{d\Psi(x,t)}{dx} = \frac{iP_x}{\hbar}\Psi(x,t)$ —— (V)

Again, differentiating partially w.r.t. x, we get,

$$\frac{\partial}{\partial x}\left(\frac{\partial\Psi(x,t)}{\partial x}\right) = \left(\frac{iP_x}{\hbar}\right)\cdot\frac{\partial\Psi(x,t)}{dx}$$

$$\frac{\partial^2\Psi(x,t)}{\partial x^2} = \left(\frac{iP_x}{\hbar}\right)\times\left(\frac{iP_x}{\hbar}\right)\cdot Ae^{i(P_x/\hbar\, x - E/\hbar\, t)}$$

[using eqⁿ (V)]

or, $\frac{\partial^2\Psi(x,t)}{\partial x^2} = \frac{-P_x^2}{\hbar^2}\Psi(x,t)$

or, $\frac{\hbar^2\partial^2\Psi(x,t)}{\partial x^2} = -P_x^2\Psi(x,t)$

Dividing both sides by $2m$,

$$\frac{\hbar^2\partial^2\Psi(x,t)}{2m\cdot\partial x^2} = \frac{-P_x^2}{2m}\cdot\Psi(x,t)$$

or, $\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} = \frac{P_x^2}{2m}\cdot\Psi(x,t)$ —— (VI)

Again, differentiating eqⁿ (IV) partially w.r.t. 't', we get,

$$\frac{\partial\Psi(x,t)}{\partial t} = Ae^{i\left(\frac{P_x}{\hbar}\times x - \frac{E}{\hbar}\times t\right)} \times\left(\frac{-iE}{\hbar}\right)$$

or, $\frac{\partial\Psi(x,t)}{\partial t} = \Psi(x,t)\times\left(-\frac{iE}{\hbar}\right)$ [using eqⁿ (IV)]

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$$or, -\frac{\hbar^2}{i} \times \frac{\partial \Psi(x,t)}{\partial t} = E\Psi(x,t)$$

$$or, \frac{-\hbar i}{i \times i} \cdot \frac{\partial \Psi(x,t)}{\partial t} = E\Psi(x,t) \quad \text{--- (VII)}$$

$$or, i\hbar \frac{\partial \Psi(x,t)}{\partial t} = E\Psi(x,t) \quad \text{--- (VII)}$$

For non-relativistic particle,

$$E = K.E + P.E$$

$$= \frac{P_x^2}{2m} + V_x$$

$$or, E\Psi(x,t) = \frac{P_x^2}{2m} \Psi(x,t) + V_x \Psi(x,t)$$

Using eqn (VI) and (VII), we get

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V_x \Psi(x,t)$$

$$or, i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_x \right) \Psi(x,t) \quad \text{--- (VIII)}$$

This is schrodinger's time dependent eqn.

Now, for schrodinger time independent eqn. we have,

Schrodinger's Time Dependent wave equation

$$i\hbar^2 \frac{\partial \Psi(x,t)}{\partial t}$$

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In 3-D,

$$\frac{i\hbar \Psi(r,t)}{\partial t} = \left(\frac{-\hbar^2}{2m}\nabla^2 + V_r\right)\Psi(r,t)$$

This is the schrodinger's time dependent wave eq^n.

Now,
for schrodinger's time independent eq^n.
We have,
schrodinger's Time dependent wave equation.

$$\frac{i\hbar\,\partial(r,t)}{\partial t} = \left(\frac{-\hbar^2}{2m}\nabla^2 + V_r\right)\Psi(r,t) \quad \text{--- (i)}$$

Suppose, $\Psi(r,t) = \phi(t)\cdot\Psi(r)$ --- (ii)

Using eq^n (ii) in eq^n (i) we get;

$$\therefore \frac{i\hbar\,\partial\{\phi(t)\cdot\Psi(r)\}}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_r\right]\phi(t)\cdot\Psi(r)$$

or, $$\Psi(r)\,\frac{i\hbar\,\partial\{\phi(t)\}}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\{\phi(t)\cdot\Psi(r)\} + V_r\{\phi(t)\cdot\Psi(r)\}$$

or, $$\Psi(r)(i\hbar)\frac{\partial\{\phi(t)\}}{\partial t} = \phi(t)\left[-\frac{\hbar^2}{2m}\nabla^2\Psi(r) + V_{(r)}\cdot\Psi(r)\right]$$

Dividing both sides by $\phi(t)\cdot\Psi(r)$,

$$\frac{i\hbar}{\phi(t)}\cdot\frac{\partial\phi(t)}{\partial t} = \frac{1}{\Psi(r)}\left[-\frac{\hbar^2}{2m}\nabla^2\Psi(r) + V_{(r)}\cdot\Psi(r)\right] = E \quad \text{(iii)}$$

function of time ≠ function of r so, E

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where, E is separation constant and actually it is a total energy.

Now,

Equating last two terms of eq^n (III) we get

$$\frac{1}{\psi(r)}\left[\frac{-\hbar^2}{2m}\nabla^2\psi(r) + V_r\,\psi(r)\right] = E$$

$$\therefore \boxed{E\cdot\psi(r) = \frac{-\hbar^2}{2m}\nabla^2\psi(r) + V_r\,\psi(r)} \quad \text{— (IV)}$$

This is the schrodinger's time independent wave equation.

It is second order linear homogenous partial differential equation.

Note (for knowledge)

for solution of $\phi(t)$;

Equating first & last terms of eq^n (III), we get

$$E = \frac{i\hbar}{\phi(t)}\frac{\partial\phi(t)}{\partial(t)}$$

$$\frac{\partial\phi(t)}{\phi t} = \frac{E\,\phi(t)}{i\hbar}$$

$$\text{or, } \frac{\partial\phi(t)}{\phi(t)} = \frac{-iE\,\partial(t)}{\hbar}$$

Integrating both sides.

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$$\int \frac{\partial \phi(t)}{\phi(t)} = \int -\frac{iE}{\hbar}\, \partial(t)$$

or, $\boxed{\ln\{\phi(t)\} = \frac{-iEt}{\hbar} + c}$ —— (V)

for $t=0$,

$$\ln \phi(0) = 0 + c$$

$$\therefore \boxed{c = \ln \phi(0)} \text{ —— (VI)}$$

Using eqn (VI) ~~and~~ in eqn (V) we get

$$\boxed{\ln \phi(t) = \frac{-iEt}{\hbar} + \ln \phi(0)}$$

or, $\ln \phi(t) - \ln \phi(0) = \frac{-iEt}{\hbar}$

$[\because \ln x = y,\ x = e^y]$

or, $\ln\left(\frac{\phi(t)}{\phi(0)}\right) = \frac{-iEt}{\hbar}$

or, $\frac{\phi(t)}{\phi(0)} = e^{-iEt/\hbar}$

$$\therefore \boxed{\phi(t) = \phi(0) \cdot e^{-\frac{iEt}{\hbar}}} \text{ —— (VII)}$$

This is the solution for $\phi(t)$.

for solution of $\psi(r,t)$;

$$\psi(r,t) = \phi(t) \cdot \psi(r)$$

$$\psi(r,t) = \phi(0) \cdot e^{-\frac{iEt}{\hbar}} \cdot \psi(r) \text{ —— (VIII)}$$

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for solution of $\psi(r)$:

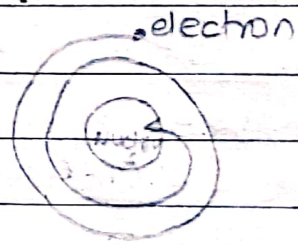
It is obtained by solving schrodinger's time independent wave equation.

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V_r \psi(r) = E \psi(r).$$

* Inadequacy of classical mechanics (Drawbacks)
(Necessity of quantum mechanics)

1) Classical mechanics can't explain stability of atom.

Explanation: According to classical Mechanics accelerating charged particle looses energy in the form of electromagnetic radiation.
Thus electron revolving around nucleus also must lose energy and consequently its radius decreases gradually and finally collapses into the nucleus. This shows instability of atom.



2) Classical Mechanics can't explain observed discrete atomic spectra.

3) Classical Mechanics can't explain photoelectric effect.
According to classical Mechanics, kinetic energy of emitted electron depends upon intensity of incident radiation but experimental result shows that K.E is ~~de~~ independent of intensity and only depends upon frequency of incident radiation.

Note:

$$hf = \phi + K.E$$
$$K.E = (hf - \phi)$$

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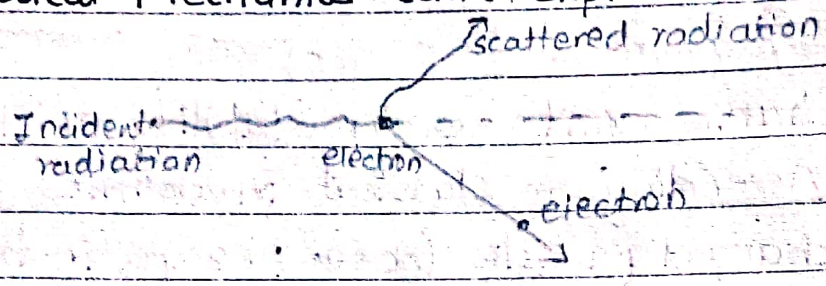
4) Classical Mechanics can't explain compton effect.



According to classical mechanics, wavelength of scattered radiation must be same with the wavelength of incident radiation but experimental result shows that these two wavelengths are not equal.

i.e. change in wavelength $(\Delta\lambda) = 0$ (classical mechanics)

$\Delta\lambda \neq 0$ (Quantum mechanics)

$$\boxed{\Delta\lambda = \frac{h}{m_0 c}(1-\cos\theta)}$$

where, θ = ~~sta~~ scattering angle.

m_0 = rest mass of electron $(9.1 \times 10^{-31} kg)$

5. Classical Mechanics fails to explain heat capacity of solids at low temperature.

6. Classical mechanics fails to explain super conductivity, anomalous zeeman effect, Raman effect, stark effect, etc.

7. Classical mechanics fails to explain black body spectrum.

8. Classical mechanics fails to explain Radioactivity such as α-decay.

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Wave Function

Physical interpretation of wave function

Wave function (ψ) is obtained by solving scrodingers wave equation and generally it is a complex number and hence direct physical meaning of wave function is not possible. However if we multiply wave function (ψ) by its complex conjugate (ψ^*) then we obtain a real and positive number. This real and positive number ($\psi^* \psi$) is known as probability density and is helpful to find probability of finding a particle in a given region of space.

Here,

$\boxed{\psi = a + ib}$, $\underbrace{\text{where 'a' and 'b' are real number}}$ — complex number

&

$\boxed{\psi^* = a - ib}$

Now,

$$\psi\psi^* = (a+ib)(a-ib)$$
$$= a^2 - (ib)^2$$
$$= a^2 + b^2 \text{ real and positive number.}$$

Properties of valid wave function

i) It must be single valued. $|z|^2 = z \cdot z^*$

ii) It must be square integrable

i.e. $\iiint \psi^* \psi \, dv = \text{finite}$ or, $\iiint |\psi|^2 dv = \text{finite}$

iii) It must be continuous.

iv) It must be finite.

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Normalization

Normalization is the process of fixing amplitude of wave function.

For example:

Suppose wave function ψ is not normalized in given region of space and normalized wavefunction is,

$$\boxed{\psi_N = A\psi} \quad \text{--- (1)}$$

where,

A is known as normalization constant.

$\because$ Particle is sure to find in a ~~infinite re~~ entire region of space.

Total probability = 1.

$$\boxed{\iiint \psi_N^* \psi_N \, dV = 1} \quad \text{--- (2)}$$

This is called normalization condition.

~~Using eq^n (1)~~

Calculation for normalization constant,

Using eq^n (1) and (2), we get,

$$\iiint (A\psi)^* (A\psi) \, dv = 1$$

$$\text{or, } \iiint (A^* \psi^*)(A\psi) \, dv = 1$$

$$\text{or, } \iiint |A|^2 \cdot \psi^* \psi \, dv = 1$$

$$\text{or, } |A|^2 \iiint \psi^* \psi \, dv = 1$$

or, $\boxed{|A|^2 = \dfrac{1}{\iiint \psi^* \psi \, dv}}$

We can calculate normalization constant (A) from this relation.

Q. A particle is confined in a 1-dimensional box and its wave function is $\psi(x) = \sin\left(\frac{n\pi}{l}\right)x$ for $0 \le x \le l$.

$= 0$ (otherwise)

Find ① Normalization constant
(ii) Normalized wave function.

Soln :

Given,

$$\psi(x) = \sin\left(\frac{n\pi}{l}\right)x \quad \text{for } 0 \le x \le l$$

$$= 0 \quad \text{otherwise.}$$

Suppose normalized wave function is,

$$\psi_N = A\psi$$

$$\boxed{\psi_N = A \cdot \sin\left(\frac{n\pi}{l}\right)x}$$

where, A is normalization constant.

Using normalization condition.

$$\int \psi_N^* \psi_N \, dx = 1$$

$$\cancel{\int_{-\infty}^{0} \psi_N^* \psi_N \, dx}^{\,0} + \int_0^l \psi_N^* \psi \, dx + \cancel{\int_l^{\infty} \psi_N^* \psi_N \, dx}^{\,0} = 1$$

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$$\int_0^l \psi_N^* \psi_N = 1$$

or, $\int_0^l \left(A \sin \frac{n\pi}{l} x\right) \left(A \sin \frac{n\pi}{l} x\right) dx = 1$

or, $\int_0^1 |A|^2 \sin^2 \frac{n\pi}{l} x \, dx = 1.$

or, $A^2 \int_0^l \sin^2 \frac{n\pi}{l} x \, dx = 1$

or, $A^2 \int_0^l \frac{1 - \cos\left(\frac{2n\pi}{l} x\right)}{2} dx$ ⟵ $\sin^2 x = \frac{1 - \cos 2x}{2}$

$\cos 2A = 1 - 2\sin^2 A$

or, $\frac{A^2}{2} \left[\int_0^l dx - \int_0^l \cos\left(\frac{2n\pi}{l} x\right) dx \right] = 1$

or, $\frac{A^2}{2} \quad [x]_0^l - \cancel{\left[\frac{\sin\left(\frac{2n\pi}{l} x\right)}{\left(\frac{2n\pi}{l}\right)} \right]_0^1} = 1.$

or, $\frac{A^2}{2} [l] = 1$

or, $A^2 = \frac{2}{l}$

or, $\boxed{A = \sqrt{\frac{2}{l}}}$

$\therefore$ normalization constant is $\sqrt{\frac{2}{l}}$.

(ii) Normalization wavefunction,

$$\psi_N(x) = A \psi(x)$$

$$= \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi}{l}\right) x \quad \text{for } 0 \le x \le l.$$

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* Note

① Schrodinger's time independent wave equation.

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

multiplying both sides by $\left(\frac{-2m}{\hbar^2}\right)$

$$\nabla^2\psi - \frac{2mV}{\hbar^2}\psi = -\frac{2m}{\hbar^2}E\psi$$

or, $$\nabla^2\psi + \frac{2mE}{\hbar^2}\psi - \frac{2mV}{\hbar^2}\psi = 0$$

or, $$\boxed{\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0}$$

where,

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

In 1-dimension,

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

If $\psi = \psi(x)$,

$$\frac{\partial\psi}{\partial x} = \frac{d\psi}{dx}$$

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2} = \frac{d^2\psi}{dx^2}$$

Now, schrodinger's time independent wave equation can be in 1-dimension can be written as,

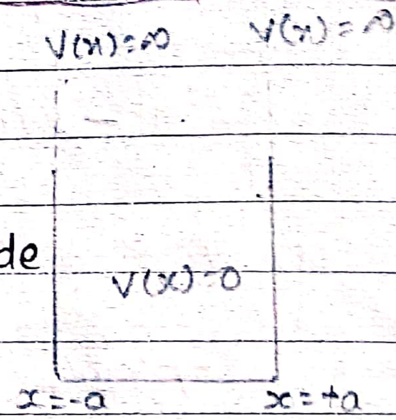
$$\boxed{\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi(x) = 0}$$

(11) $\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$

$\psi(x) = A\sin kx + B\cos kx.$

* Applications of Schrodinger's ~~wave~~ time independent wave equation:

1) Particle inside one-dimensional box.



consider a particle of mass 'm' is inside one-dimensional box of.

$V_x = 0$ if $-a < x < a$

$= \infty$ otherwise.

We have schrodinger's time independent wave equation in 1-dimension.

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V_x)\psi(x) = 0.$$

Using $V_x = 0$, we get,

$$\frac{d^2\psi(x)}{dx^2} + \left(\frac{2m}{\hbar^2}E\right)\psi(x) = 0$$

or, $$\boxed{\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0} \quad \text{--- (1)}$$

where,

$k^2 = \frac{2mE}{\hbar^2}$ — (2) is real and positive number.

We know solution of eq^n (1) is,

$$\boxed{\psi(x) = A\sin kx + B\cos kx} \quad \text{--- (3)}$$

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$\because$ Wave function $\psi(x)$ vanishes at a region of infinite potential energy.

$$\psi(x)\Big|_{x=-a} = 0 \quad \text{and} \quad \psi(x)\Big|_{x=+a} = 0$$

$$\because \psi(x)\Big|_{x=-a} = 0.$$

$$\Rightarrow A\sin k(-a) + B\cos k(-a) = 0$$

$$\boxed{-A\sin ka + B\cos ka = 0} \quad \text{---} (4)$$

$$\because \psi(x)\Big|_{x=+a} = 0$$

$$\boxed{A\sin ka + B\cos ka = 0} \quad \text{---} (5)$$

Now,

adding eq^n (4) and (5) we get.

$$2B\cos ka = 0$$

$$B\cos ka = 0 \quad \text{---} (6)$$

Subtracting eq^n (4) from (5)

$$2A\sin ka = 0$$

$$A\sin ka = 0 \quad \text{---} (7)$$

from eq^n (6)

$$\cos ka = 0 \quad \text{if } B \neq 0$$

$$\cos ka = \cos\frac{\pi}{2}, \cos\frac{3\pi}{2}, \cos\frac{5\pi}{2}, \ldots$$

$$ka = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots$$

$$\boxed{k = \frac{n\pi}{2a}} \quad \text{---} (8) \quad \text{where, } n = 1, 3, 5, 7, \ldots$$

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from eqn ⑦

$\sin ka = 0$ if $A \neq 0$.

$\sin ka = \sin \frac{2\pi}{2}, \sin \frac{4\pi}{2}, \ldots$

$ka = 2\left(\frac{\pi}{2}\right), 4\left(\frac{\pi}{2}\right), \ldots$

$ka = n\frac{\pi}{2}$, $n = 2, 4, 6, \ldots$

$$\boxed{k = \frac{n\pi}{2a}} \quad \text{—— ⑨ where } n = 2, 4, 6, \ldots$$

from eqn ⑧ and ⑨, we get

$$\boxed{k = \frac{n\pi}{2a}} \quad \text{—— ⑩ where } n = 1, 2, 3, 4, 5, \ldots$$

Now, using eqn ⑩ in eqn ②, we get.

$$\left(\frac{n\pi}{2a}\right)^2 = \frac{2mE}{\hbar^2}$$

or, $E = \frac{\hbar^2}{2m}\left(\frac{n\pi}{2a}\right)^2$, ~~n = 1, 2, 3, ...~~

In general,

$$\boxed{E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{2a}\right)^2} \quad \text{—— ⑪}$$

For $n = 1$ (Ground state)

$E_1 = \frac{\hbar^2}{2m}\left(\frac{n\pi}{2a}\right)^2$

$\therefore \boxed{E_n = n^2 \cdot E_1}$

For $n=2$ (1^{st} excited state),

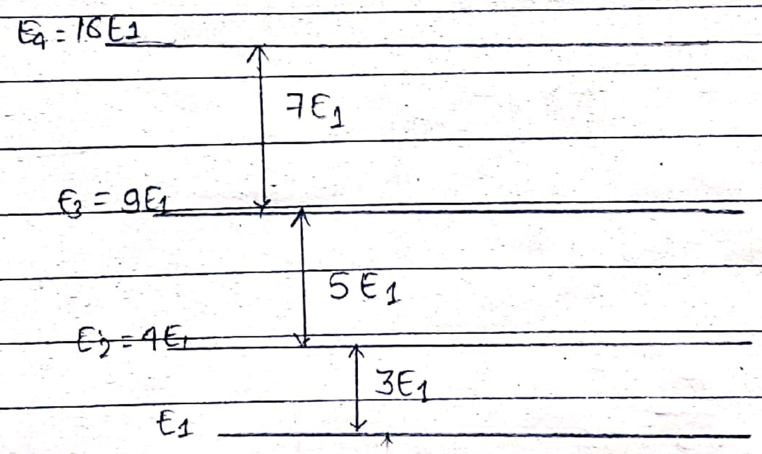
$$E_2 = 2^2 \cdot E_1 = 4E_1.$$

For $n=3$ (2^{nd} excited state),

$$E_3 = 9E_1$$

For $n=4$ (3^{rd} excited state),

$$E_4 = 16E_1$$



Now, wavefunction,

$$\psi(x) = A \sin kx \qquad , n = 2, 4, 6, \ldots$$

and $$\psi(x) = B \cos kx \qquad , n = 1, 3, 5, \ldots$$

For A,

Using normalization condition,

$$\int_{-a}^{a} \psi^* \psi \, dx = 1$$

or, $$\int_{-a}^{a} (A \sin kx)^* (A \sin kx) \, dx = 1$$

or, $A^2\int_{-a}^{a}\sin^2 kx\,dx = 1.$

or, $A^2\int_{-a}^{a}\left(\frac{1-\cos 2kx}{2}\right)dx = 1$

or, $\frac{A^2}{2}\left[\int_{-a}^{a}1\,dx - \int_{-a}^{a}\cos 2kx\,dx\right] = 1$

$k = n\pi/2a$

or, $\frac{A^2}{2}\left[[x]_{-a}^{a} - \cancel{\left[\frac{\sin 2kx}{2k}\right]_{-a}^{a}}\right] = 1$

$\left(\frac{\sin 2kx}{2k}\right)_{a}^{-a}$

$\frac{\sin 2ka + \sin 2ka}{2k}$

$\frac{\sin 2\cdot\frac{n\pi}{2a}a + \sin\frac{2n\pi}{2a}a}{2k}$

$\xrightarrow{} 0$ $\frac{\cancel{\sin n\pi} + \sin n\pi}{2k}$

or, $\frac{A^2}{2}\times 2a = 1$

or $A^2 = \frac{1}{a}$

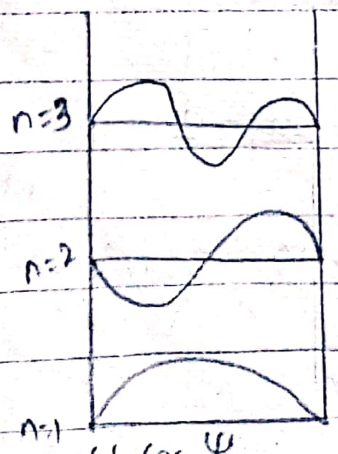
or, $\boxed{A = \frac{1}{\sqrt{a}}}$

Similarly, $B = \frac{1}{\sqrt{b}}$

$\therefore$ Normalized wave function,

$\psi(x) = A\sin kx = \frac{1}{\sqrt{a}}\sin\frac{n\pi}{2a}x, \quad n = 2, 4, 6, \dots$

$\psi(x) = B\cos kx = \frac{1}{\sqrt{a}}\cos\frac{n\pi}{2a}x, \quad n = 1, 3, 5, 7, \dots$



plot for ψ

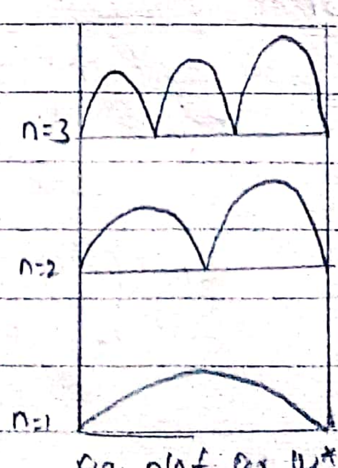
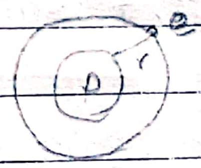


fig: plot for $\psi^*\psi$

* Solution of Hydrogen atom

Wrong



Consider an electron of charge $(-e)$ is revolving around nucleus in a circular path of radius 'r' then

potential energy,

$$V(r) = \frac{1}{4\pi\epsilon_0}\frac{(+e)(-e)}{r} \qquad \left[\because PE = \frac{1}{4\pi\epsilon_0}\frac{q_1 q_2}{r}\right]$$

$$V(r) = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

We have,
Schrondinger's time independent wave equation in 3-D,

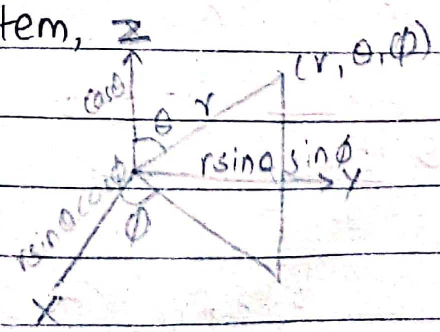
$$\nabla^2 \psi + \frac{2\mu}{\hbar^2}(E-V)\psi = 0 \quad \text{--- (1)}$$

where, μ = Reduced mass

$$= \frac{m_p \times m_e}{m_p + m_e}$$

where, m_p = mass of ~~electron~~ proton.
m_e = mass of electron.

In spherical polar coordinate system,



not necessary

$x = r\sin\theta\cos\phi$

$y = r\sin\theta\sin\phi$

$z = r\cos\theta$

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Using these in eq^n ① we can write schrodinger time independent equation in spherical polar coordinate system.

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$
$$+\frac{2\mu}{\hbar^2}(E-V_r)\psi=0 \quad \text{——— ②}$$

Here, $\psi=\psi(r,\theta,\phi)$.

Using method of separation of variables,

$$\psi(r,\theta,\phi)=R(r)\,\Theta(\theta)\,\Phi(\phi) \quad \text{——— ③}$$

using ③ in ②,

$$\Theta(\theta)\Phi(\phi)\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)+\frac{1}{r^2\sin\theta}R(r)\Phi(\phi)\frac{\partial}{\partial\theta}\left(\frac{\sin\theta\,\partial\Theta(\theta)}{\partial\theta}\right)$$
$$+\frac{1}{r^2\sin^2\theta}R(r)\Theta(\theta)\frac{\partial^2\Phi(\phi)}{\partial\phi^2}+\frac{2\mu}{\hbar^2}(E-V(r))R(r)\Theta(\theta)\Phi(\phi)=0$$

Dividing by $R(r)\,\Theta(\theta)\,\Phi(\phi)$; we get.

$$\frac{1}{R(r)}\frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{r^2\partial R(r)}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{1}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left(\frac{\sin\theta\,\partial\Theta(\theta)}{\partial\theta}\right)$$
$$+\frac{1}{r^2\sin^2\theta}\frac{1}{\Phi(\phi)}\frac{\partial^2\Phi(\phi)}{\partial\phi^2}+\frac{2\mu}{\hbar^2}(E-V(r))=0$$

$$\frac{1}{R(r)}\frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{r^2\partial R(r)}{\partial r}\right)+\frac{2\mu}{\hbar^2}(E-V(r))=$$

Multiplying both sides by r^2, we get

$$\frac{1}{R(r)}\frac{\partial}{\partial r}\left(\frac{r^2\partial R(r)}{\partial r}\right)+\frac{1}{\sin\theta}\frac{1}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left(\frac{\sin\theta\,\partial\Theta(\theta)}{\partial\theta}\right)$$

$$+\frac{1}{\sin^2\theta}\cdot\frac{1}{\Phi(\theta)}\frac{\partial^2\Phi(\phi)}{\partial\phi^2}+\frac{2\mu r^2}{\hbar^2}(E-V(r))=0$$

or, $$\frac{1}{R(r)}\frac{\partial}{\partial r}\left(\frac{r^2\partial R(r)}{\partial r}\right)+\frac{2\mu r^2}{\hbar^2}(E-V(r))=$$

$$-\frac{1}{\sin\theta}\frac{1}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left(\frac{\sin\theta\,\partial\Theta(\theta)}{\partial\theta}\right)-\frac{1}{\sin^2\theta}\frac{1}{\Phi(\theta)}\frac{\partial^2\Phi(\theta)}{\partial\phi^2}$$

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Solution of (Hydrogen atom)

We have, ~~shcrodi~~ schrodinger time independent wave equation in spherical polar coordinates,

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} +$$

$$\frac{2\mu}{\hbar^2}(E-V(r))\psi = 0 \quad \text{--- (1)}$$

where, μ = Reduced mass = $\frac{m_e \times m_p}{m_e + m_p}$

m_e = mass of electron

m_p = mass of proton

$$V(r) = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

Here,

$$\psi = \psi(r,\theta,\phi).$$

Using method of separation of variables.

suppose,

$$\psi = R(r)\,Y(\theta,\phi) \quad \text{--- (2)}$$

Using eq^n (2) in (1) we get.

$$Y\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right) + \frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} + \frac{2\mu(E-V_r)}{\hbar^2}\times R\times Y = 0$$

Dividing both sides by RY,

$$\frac{1}{R}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{1}{Yr^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta\, Y}\frac{\partial^2 Y}{\partial\phi^2} +$$

$$\frac{2\mu(E-V_r)}{\hbar^2} = 0$$

Multiplying both sides by r^2.

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{Y\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}+\frac{2\mu r^2(E-V_r)}{\hbar^2}=0$$

or, $$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2\mu r^2(E-V_r)}{\hbar^2}=-\frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{dY}{\partial\theta}\right)-\frac{1}{Y\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}$$

or, $$\underbrace{\frac{1}{R}\frac{\partial}{\partial r}\left(\frac{r^2\partial R}{\partial r}\right)+\frac{2\mu r^2(E-V_r)}{\hbar^2}}_{\text{only depends on } r \text{ (Radial part)}}=\underbrace{-\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\frac{\sin\theta\, dY}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right]}_{\text{only depends upon } \theta \text{ and } \phi \text{ (Angular Part)}}=\lambda \text{ (suppose)} \quad (3)$$

Equating ~~(1) and (3)~~ first and last term of eq^n (3), we get

$$\frac{1}{R}\frac{\partial}{\partial r}\left(\frac{r^2\partial R}{\partial r}\right)+\frac{2\mu r^2}{\hbar^2}(E-V_r)=\lambda.$$

Dividing both sides by r^2

$$\frac{1}{R}\times\frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{r^2\partial R}{\partial r}\right)+\frac{2\mu}{\hbar^2}(E-V_r)=\frac{\lambda}{r^2}$$

or, $$\frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{r^2\partial R}{\partial r}\right)+\frac{2\mu}{\hbar^2}(E-V_r)\times R=\frac{\lambda}{r^2}\times R.$$

or, $$\frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{r^2\partial R}{\partial r}\right)+\left(\frac{2\mu}{\hbar^2}(E-V_r)-\frac{\lambda}{r^2}\right)R=0 \quad \text{— (4)}$$

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This is called radial equation.

Equating last two terms of eqn ③,

$$-\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right]=\lambda$$

or, $$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{dY}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}=-\lambda Y \quad \text{—— ⑤}$$

~~or,~~ Again, suppose

$$Y = Y(\theta,\phi)$$

$$Y = \Theta(\theta)\cdot\Phi(\phi)$$

$$\boxed{Y = \Theta\Phi} \quad \text{—— ⑥}$$

Using eqn ⑥ in eqn ⑤, we get,

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{d\Theta\Phi}{d\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\Theta\Phi}{\partial\phi^2}=-\lambda\Theta\Phi$$

or, $$\frac{\Phi}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{d\Theta}{d\theta}\right)+\frac{\Theta}{\sin^2\theta}\frac{\partial^2\Phi}{\partial\phi^2}=-\lambda\Theta\Phi.$$

Dividing both sides by $\Phi\Theta$.

or, $$\frac{1}{\Theta\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{d\Theta}{d\theta}\right)+\frac{1}{\Phi\sin^2\theta}\cdot\frac{\partial^2\Phi}{\partial\phi^2}=-\lambda$$

Multiplying both sides by $\sin^2\theta$.

$$\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{d\Theta}{d\theta}\right)+\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2}=-\lambda\sin^2\theta.$$

$$\underbrace{\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\lambda\sin^2\theta}_{\text{only function of }\theta\ (\theta\text{ part})}=\underbrace{-\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2}}_{\text{only function of }\phi\ (\phi\text{ part})}=m^2\ (\text{suppose})$$

Equating last two term of eqn ⑦, (azimuthal equation) we get,

$$-\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2} = m^2$$

or, $$\boxed{\frac{\partial^2\Phi}{\partial\phi^2} + m^2\Phi = 0}$$

This can be solved for Φ

$$\boxed{\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}}$$

where, m is magnetic quantum number.

Equating first and last ~~two~~ two term of eqn ⑦.

$$\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \lambda\sin^2\theta = m^2$$

$$\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right.$$

Solving this equation, we found Θ and new quantum number 'l' is introduced.

where, l is orbital quantum number.

solving radial eqn ④ we get R(r) and energy $E = \frac{-me^4}{8\epsilon_0^2 n^2 h^2}$

This shows that new quantum number 'n' is introduced.

where, n is called Principal quantum number.

$n = 1, 2, 3, \ldots$

—⑧ $l = 0, 1, 2, \ldots (n-1)$

$m = -l$ to $+l$ including 0.

$= 0, \pm 1, \pm 2 \ldots \pm l$.

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Significance

Physical meaning of quantum numbers

Wave function ψ of hydrogen atom depends upon three quantum number (n).

① Principal quantum number (n)
⑪ Orbital quantum number (l)
⑪ magnetic quantum numer (m)

or

magnetic orbital quantum number.

① Principal quantum number (n)

Principal quantum number is obtained by solving radial equation of H-atom. This quantum number describes the quantization of energy in H-atom.

i.e,

$$E_n = \frac{-me^4}{8\epsilon_0^2 n^2 h^2}$$

only certain discrete negative values of energy are possible as n = 1, 2, 3, ---

⑪ Orbital quantum number (l)

orbital quantum number is obtained on solving polar equation (Θ equation) of hydrogen atom and gives orbital ~~number~~ angular momentum of electron i.e,

$$L = \hbar\sqrt{l(l+1)}$$

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where,

L = orbital angular momentum

$\hbar = \frac{h}{2\pi}$

l = orbital quantum number.

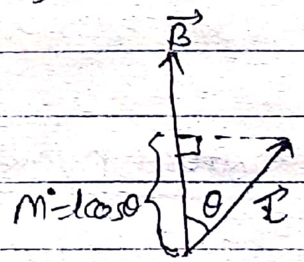
$= 0, 1, 2, \ldots (n-1)$

(iii) Magnetic Orbital quantum number (m)

This quantum number explain space quantization and is obtained on azimutal (Φ) equation of hydrogen atom.

Actually, it is the projection of orbital quantum number (l) along the direction of magnetic field i.e,

$$\boxed{m = l\cos\theta}$$

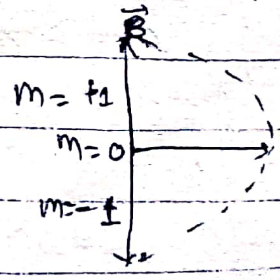


Here, ~~math~~ arithmetically,

$\cos\theta$ can have all possible values between -1 to $+1$ & if so, magnetic quantum number has infinite number of values but due to space quantization 'l' can't orient in all possible direction & hence m has only $(2l+1)$ values.

for $l = 1$,

$m = +1, 0, -1$



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Similarly, for $l=2$.
m has $(2l+1) = 5$ values.
i.e, $m = +2, +1, 0, -1, -2$.

* Pauli exclusion Principle

Statement: Only one electron can exist in a single quantum state. Quantum state of electron is given by four quantum numbers.

(i) Principal quantum number (n)
(ii) orbital quantum number (l)
(iii) magnetic orbital quantum number (m_l)
(iv) magnetic spin quantum number (m_s)

quantum state $= (n, l, m_l, m_s)$

(i) Principal quantum number

$n = 1, 2, 3, 4, \ldots$
$n=1$ (K shell)
$n=2$ (L shell)
$n=3$ (M shell)
and so on.

According to $(2n^2)$ law,
$n=1$ (K shell contains) two electrons.
$n=2$ (L-shell contains eight electron.
$n=3$ (M-shell contains eighteen electrons
and so on.

(ii) Orbital quantum number (l)

$l = 0, 1, 2, \ldots (n-1)$ — No. of eletron

		No. of eletron
$l=0$	(s-orbital) ~~No.~~	2
$l=1$	(p-orbital)	6
$l=2$	(d-orbital)	10
$l=3$	(f-orbital)	14

and so on.

(iii) magnetic orbital quantum number (m_l)

m_l has $(2l+1)$ values from $-l$ to $+l$ including zero.

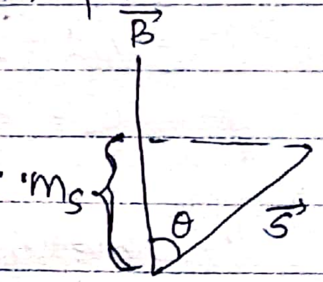
For eg:-

$l=3$, $m_l = -3, -2, -1, 0, 1, 2, 3$ (7 values).

(iv) magnetic spin quantum number (m_s)

It is a projection of spin quantum number along direction of magnetic field.

i.e, $m_s = s\cos\theta$.

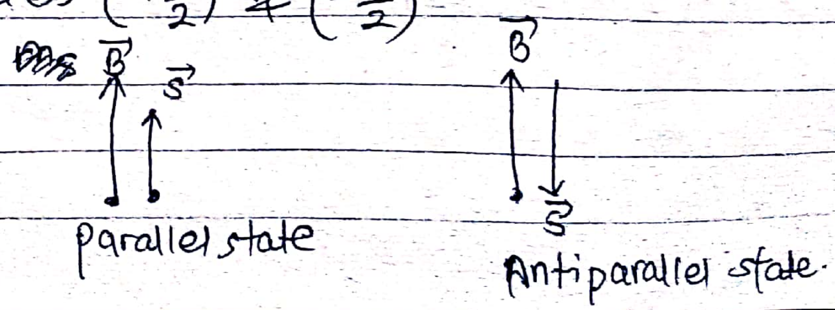


where,

s = spin quantum number.

$= \frac{1}{2}$ (for electron)

Due to space quantization, m_s have ~~eta~~ only two values $(+\frac{1}{2})$ & $(-\frac{1}{2})$



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⇒ For $n=1$ (according to $2n^2$ law)
total number of electron $=2$.
$l=0$
$m_l=0$
$m_s=+1/2, -1/2$

Here, quantum state are
(n, l, m_l, m_s)
$=(1,0,0,1/2)$ & $(1,0,0,-1/2)$

Clearly, there exists two electrons in two quantum states' i.e one electron in one quantum state.

⇒ For $n=2$ (according to $2n^2$ law).
total number of electron $=8$
$l=0,1$
for $l=0$, $m_l=0$
for $l=1$, $m_l=+1,0,-1$
$m_s=+\frac{1}{2}, -\frac{1}{2}$

Possible quantum states are,
(n, l, m_l, m_s)
$=(2,0,0,1/2)$, $(2,0,0,-1/2)$, $(2,1,+1,1/2)$,
$(2,1,+1,-1/2)$, $(2,1,0,1/2)$, $(2,1,0,-1/2)$,
$(2,1,-1,1/2)$ $(2,1,-1,-1/2)$

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For $n=3$ (M shell)

According $2n^2$ rule,

total number of electrons in M-shell is 18.

According to Pauli's exclusion Principle, there must be 18 different quantum states.

$l = 0, 1, 2$

for $l=0$, $m_l=0$

for $l=1$, $m_l = 1, 0, -1$

for $l=2$, $m_l = 2, 1, 0, -1, -2$.

$m_s = +\frac{1}{2}, -\frac{1}{2}$

Now,

18 quantum states

(n, l, m_l, m_s)

$= (3,0,0,\frac{1}{2}), (3,0,0,-\frac{1}{2}), (3,1,1,\frac{1}{2}), (3,1,1,-\frac{1}{2}),$
$(3,1,0,\frac{1}{2}), (3,1,0,-\frac{1}{2}), (3,1,-1,\frac{1}{2}), (3,1,-1,-\frac{1}{2}),$
$(3,2,2,\frac{1}{2}), (3,2,2,-\frac{1}{2}), (3,2,1,\frac{1}{2}), (3,2,1,-\frac{1}{2}),$
$(3,2,0,\frac{1}{2}), (3,2,0,-\frac{1}{2}), (3,2,-1,\frac{1}{2}), (3,2,-1,-\frac{1}{2})$
$(3,2,-2,\frac{1}{2})$ $(3,2,-2,-\frac{1}{2})$

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* Degeneracy in Hydrogen atom

If there are more than one independent wave function for single value of energy then these independent wave functions are called degenerate states and process is called degeneracy.

In H-atom, there is n^2 fold degeneracy

For example:

Energy of hydrogen atom,

$$E_n = -\frac{me^4}{8\epsilon_0^2 n^2 h^2}$$

i.e. energy depends upon principal quantum number 'n'.

But wave function, ψ depends upon three quantum number n, l and m.

i.e $\boxed{\psi = \psi_{nlm}}$

For $n = 1$,

Energy $E = E_1$

wave function $\psi = \psi_{nlm}$

$= \psi_{100}$

$n=1$
$l=0$
$m=0$

This means that ground state of hydrogen atom is non-degenerate.

For, $n=2$,

Energy $E = E_2$.

wave function $\psi = \psi_{nlm}$

$= \psi_{200}$

$n=2$
$l = 1, 0$
$m = -1, 0, 1, 0$

ψ_{21-1},

ψ_{210},

ψ_{211},

There are 4 independent wave function corresponding to single energ E_2.

$\therefore$ $n = 2$ state has four fold degeneracy.

For $n=3$,

$n=3$ $l=2$ $m=2,1,0,-1,-2$
$l=1$ $m=1,0,-1$
$l=0$ $m=0$

~~$n=3$~~
~~$l=2,1,0,m$~~

Energy $E = E_3$.

wave function $\psi = \psi_{nlm}$

$= \psi_{300}$, ψ_{31-1}, ψ_{310}, ψ_{311}

ψ_{32-2}, ψ_{32-1}, ψ_{320}, ψ_{321}

ψ_{322}

There are 9 independent wave function correspo-nding to single energy E_3

$\therefore$ $n=3$ state has nine fold degeneracy.

Similarly,

There are n^2 idependent wave function corres-ponding to single Energy E_n

$\therefore$ n state has n^2 fold degeneracy.

Zeeman effect

Splitting of spectral lines in the presence of magnetic field is called zeeman effect. Zeeman effect is the best example of spatial quantization.

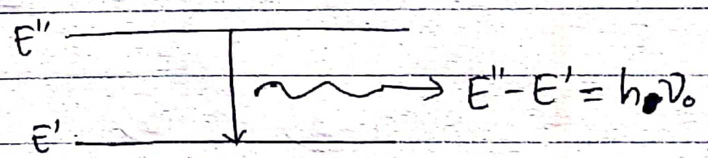
There are 2 types of Zeeman effect:

(i) Normal zeeman effect.

(ii) Anomalous Zeeman effect.

If a spectral line splits into two or three components due to presence of magnetic field then such zeeman effect is called normal zeeman effect. Similarly, if spectral line splits into more than three components then it is called anomalous zeeman effect.

Suppose



when electron falls from E'' to E' then

Energy released in the absence of magnetic field is

$E''-E' = h\nu_0$

$$\boxed{\nu_0 = \frac{E''-E'}{h}}$$

Here, ν_0 is the frequency of spectral line emitted in the absence of magnetic field.

If magnetic field 'B' is applied then emitted frequency of spectral line will be

$$\boxed{\nu = \nu_0 + \Delta\nu} \quad \text{——— (1)}$$

where, $\Delta\nu$ = change in frequency of spectral line due to magnetic field.

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$\because$ Energy $(E) = -\vec{\mu_l} \cdot \vec{B}$

$= -\mu_l B \cos\theta$

$= -\frac{eh}{4\pi m} l B \cos\theta$ $\quad \left[\because \mu_l = \frac{ehl}{4\pi m}\right]$

$E = -\frac{ehB}{4\pi m} l\cos\theta$ $\quad [m_l = l\cos\theta]$

$E = -\frac{ehB}{4\pi m} m_l$

$\Delta E = \frac{ehB}{4\pi m} \Delta m_l$

or, $\Delta(h\nu) = \frac{ehB}{4\pi m} \Delta m_l$

or, $\boxed{\Delta\nu = \frac{e\cancel{h}B}{4\pi m} \Delta m_l}$ — (2)

Using (2) in (1)

$$\boxed{\nu = \nu_0 + \frac{eB}{4\pi m} \Delta m_l}$$

Using, selection rule

$\Delta m_l = \pm 1, 0$

$\nu = \nu_0 + \frac{eB}{4\pi m}$ $\quad$ (for $\Delta m_l = +1$)

$\nu = \nu_0$ $\quad$ (for $\Delta m_l = 0$)

$\nu = \nu_0 - \frac{eB}{4\pi m}$ $\quad$ (for $\Delta m_l = -1$)

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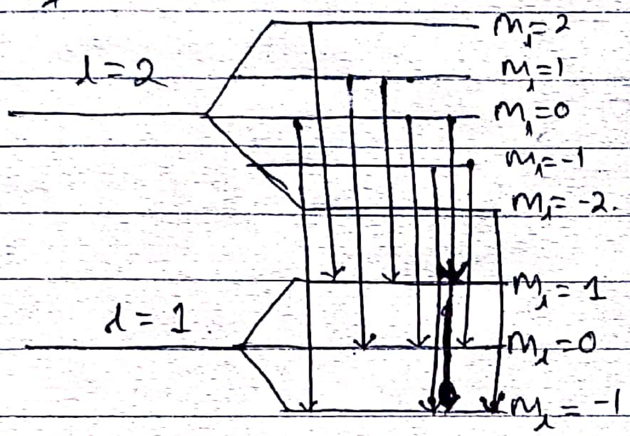
Q. Obtain possible splitting in Normal Zeeman effect when an electron undergoes transition from $l=2$ state to $l=1$ state.

Soln



shell

n=1	K
n=2	L
n=3	M
n=4	N

subshell

l=0	s
l=1	p
l=2	d
l=3	f

There are only 9 possible transitions from $l=2$ to $l=1$ due to spatial quantization ($\Delta m_l = \pm 1, 0$).

Three ~~spectral~~ transitions for $\Delta m_l = +1$.

3 transitions for $\Delta m_l = -1$

3 transitions for $\Delta m_l = 0$.

* Spin

Spin of earth means its rotation about an axis passing through its centre.

But spin of electron has nothing to do with rotation and it is an intrinsic property of material. And gives intrinsic angular momentum.

In quantum mechanics,

intrinsic angular momentum,

$$S = \hbar \sqrt{s(s+1)}$$

where, s = spin quantum number

S = Intrinsic angular momentum.

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For electron,

$$s = \frac{1}{2}$$

$$S = \hbar\sqrt{\tfrac{1}{2}\left(\tfrac{1}{2}+1\right)}$$

$$= \hbar\sqrt{\frac{1}{2}\times\frac{3}{2}}$$

$$= \hbar\sqrt{\frac{3}{4}}$$

$$= \frac{\hbar}{2}\sqrt{3}$$

* Stern - Gerlach experiment