De-Broglie waves: According to De-Broglie, a moving particle is associated with a wave whose wavelength depends upon mass and velocity of the moving particle. Such waves are called De-Broglie waves for matter waves.

According to De-Broglie:

\[ \lambda = \frac{h}{mv} = \frac{h}{p} \]

where \( h \) is Planck's constant
\[ h = 6.63 \times 10^{-34} \text{Js} \]

\( m \) = mass of moving particle,
\( v \) = velocity of moving particle,
\( p \) = momentum of moving particle.

By Planck's theory:

\[ E = \frac{hc}{\lambda} = \frac{hc}{E} = \frac{h}{mc^2} = \frac{h}{mc} \]

Here \( mc \) = momentum of photons

Hence whatever is true for a moving particle, the same theory is applied for photons.

Numerical: Calculate momentum of electrons and photons moving with velocity.
\( V = 2 \times 10^8 \text{ m/s} \)

\[
\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{9.11 \times 10^{-31} \times 9 \times 10^8}
\]

\[
\lambda = \frac{h}{mc} = \frac{6.63 \times 10^{-34}}{6.022 \times 10^{23} \times 3 \times 10^8}
\]

\[
E_k = \frac{1}{2}mv^2
\]

\[
E_k = \frac{m^2v^2}{2m} = \frac{p^2}{2m}
\]

\[
p = \sqrt{2mE_k}
\]

\[
d = \frac{h}{p} = \frac{h}{\sqrt{2mE_k}}
\]

For a particle having charge \( q \) and accelerated through potential difference \( V \),

\[
E_k = qV
\]

\[
\lambda = \frac{h}{\sqrt{2mqV}}
\]

For a particle in thermal equilibrium,

\[
E_k = \frac{3}{2} k_B T
\]
where \( k_B = \text{Boltzmann Constant} \)
\[
= 1.38 \times 10^{-23} \text{ J/K}
\]

\[
\lambda = \frac{\hbar}{13m k_B T}
\]

Wave velocity or Phase velocity :-

The velocity with which planes of constant phase propagate through the medium is known as wave velocity or phase velocity.

Or the velocity of advancement of monochromatic wave is known as wave velocity or phase velocity.

Eqn of plane progressive wave is,
\[
y = a \sin (\omega t - kx)
\]

where, \( \omega \) = angular frequency.
\[
= 2\pi \frac{y}{T}
\]

\[ l \]

\[ R = \text{propagation constant} \]
\[
= \frac{\omega}{k}
\]

Here phase of wave \( \xi \)

\( (\omega t - kx) = \text{constant} \)

Differentiating w.r.t. time
\[
\omega - R\frac{dx}{dt} = 0
\]

\[
\text{or,} \quad \frac{dx}{dt} = \frac{\omega}{R} = \omega \left(\frac{\text{phase vel.}}{v_p}\right)
\]
Dence phase velocity is the ratio of angular frequency $\omega$ to the propagation constant $k$.
\[
U = \frac{\omega}{k} = \frac{2\pi f}{\alpha}
\]

Also,
\[
E = hv
\]

or,
\[
E = \frac{c_0 e}{h}
\]

\[
\lambda = \frac{2\pi}{k}
\]

\[
E = \frac{c_0 m v}{\lambda}
\]

\[
\Omega = \frac{c_0 m v}{\lambda}
\]

\[
\Omega = \frac{c_0 m v}{c_0 m v} = \frac{c_0 m v}{c_0 m v} = \frac{c_0 m v}{c_0 m v}
\]

From above expression we find that:
\[
: \ c > \gamma v
\]

Phase velocity is greater than the velocity of light which is not possible. Hence, to overcome this problem group velocity was calculated which change no of waves were assumed to travel in single group.
Group velocity

It is the velocity with which slowly varying envelope of modulated pattern due to group of waves travel in the medium.

Consider a group of waves consisting of two components given by

\[ y_1 = a \sin (\omega_1 t - k_1 x) \quad \text{(i)} \]
\[ y_2 = a \sin (\omega_2 t - k_2 x) \quad \text{(ii)} \]

Resultant wave,

\[ y = y_1 + y_2 \]

\[ y = a \left[ \sin (\omega_1 t - k_1 x) + \sin (\omega_2 t - k_2 x) \right] \]

\[ = a \sin \left[ \omega_0 t - k_0 x \right] \]

\[ = a \sin \left[ \frac{\omega_1 + \omega_2}{2} t - \frac{k_1 + k_2}{2} x \right] \]

\[ \cos \left[ \frac{\omega_1 - \omega_2}{2} t - \frac{k_1 - k_2}{2} x \right] \]

but, \( \omega_1 - \omega_2 = \Delta \omega \) ? \( \omega_1 + \omega_2 = \omega \)

\[ k_1 - k_2 = \Delta k \]

\[ \frac{k_1 + k_2}{2} = \frac{\omega}{2} \]
\[ y = 2a \sin (\omega t - kx) \cos \left( \frac{\Delta \omega t - \Delta k x}{2} \right) \]  

Comparing eqn. (i) with eqn. (ii) and (iii), we find that the amplitude of the resultant wave is

\[ A = 2a \cos \left( \frac{\Delta \omega t - \Delta k x}{2} \right) \]

Equation (ii)

Resultant wave is superposition of two components

(i) \( \sin(\omega t - kx) \) which gives the expression for phase velocity

\[ c_\phi = v_p = \omega \]

(ii) \( \cos\left(\frac{\omega t - kx}{2}\right) \)

which will give the expression for group velocity given by

\[ c_g = \frac{\partial \omega}{\partial k} = \frac{\Delta \omega}{\Delta k} \]

\[ = \frac{\omega}{\Delta k} \]

\[ g = \frac{dw}{dk} = \frac{d}{dk} \left( \frac{2\pi}{\lambda} \right) = -\frac{1}{\lambda^2} \frac{d\lambda}{d\lambda} \]
\[ G = -\frac{1}{c^2} \frac{dv}{dt} \]

Also,
\[ W = \frac{\sigma \pi}{1} = \frac{\sigma \pi}{\lambda} \]
\[ R = \frac{\sigma \pi}{1} = \frac{\sigma \pi}{\lambda} \]
\[ \therefore \frac{W}{R} = \frac{E}{p} \]
\[ \therefore \] \[ G = \frac{dw}{dk} = \frac{dE}{dp} \]

Relation b/w group vel. and phase vel.
\[ \frac{G}{d\omega} = \frac{d}{dk} \left( \frac{d\omega}{dk} \right) \]
\[ = \omega + k \frac{d\omega}{dk} \]
\[ \therefore k = \frac{\sigma \pi}{c} \]

\[ dk = -\frac{\sigma \pi}{c^2} dt \]
\[ \therefore \frac{dk}{dt} = -\frac{1}{c} \]

put (2) in eq (3)

\[ G = \omega - \lambda \frac{d\omega}{dt} \] for dispersive medium.

or
\[ G = \omega - \lambda \frac{dv}{dt} \]
for non-dispersive medium, medium in which waves of all wavelengths travel with same speed.

\[ \frac{du}{dt} = 0 \]

\[ \Gamma = \frac{cl}{\infty} \]

\[ V_p = \sqrt{c} \]

X. Time \( T \) prove that product of \( X \) and \( \tau \).

**Relationship between phase velocity and particle velocity.**

(for non-rel. case) & (for free particle)

\[ u = \omega \tau \]

\[ \omega = 2 \pi \tau \]

\[ \omega \tau = \frac{E}{mV} \]

\[ \omega \tau = \frac{1}{2} \frac{mv^2}{mV} \]

\[ V_p = \frac{V}{2} \]

Relation btw. group vel. and particle velocity. (Non rel. case)
\[ \frac{dG}{dp} = \frac{dE}{dp} \]

Here, \( E = \frac{1}{2} m v^2 \)

\[ dE = m v \, dv \]

\[ \frac{dE}{dp} = m v \cdot dv \]

\[ \frac{G}{dp} = \frac{mv dv}{mdv} = \frac{v}{c} \]

\[ G = v \] or \[ \sqrt{G^2} = v \]

Relation between group velocity and particle velocity (in relativistic case)

\[ G = \frac{dG}{dp} = \frac{dE}{dp} \]

\[ E^2 = p^2 c^2 + mv^2 c^4 \]

\[ \frac{\partial}{\partial dp} E = \frac{\partial}{\partial dp} (p^2 c^2 + mv^2 c^4) \]

\[ \frac{\partial E}{\partial dp} = 2pc^2 dp \]

\[ \frac{dE}{dp} = \frac{pc^2}{E} = \frac{mv}{mc^2} = \frac{v}{c} \]

\[ G = \frac{dE}{dp} = \frac{v}{c} \]

\[ \sqrt{G^2} = v \]

Hence prove that the product of phase velocity and group velocity is equal to \( \sqrt{c^2} \) the speed of light.
\[ m = \frac{c^2}{v} \]
\[ \mu \times v = c^2 \]
\[ [\mu \times a = c^2] \]

**Question:** Calculate de Broglie wavelength of electron and photon each of energy \( 2 \) electronvolts.

**Solution:**

for photons

\[ \lambda = \frac{h}{E} \]

Now, a particle of rest mass \( m_0 \) has kinetic energy \( K \). Show that its de Broglie wavelength is given by

\[ \lambda = \frac{h}{\sqrt{K(K + 2m_0c^2)}} \]

**Solution:**

\[ \lambda = \frac{h}{mv} - c \]

\[ m = m_0 \]

\[ \sqrt{\frac{1 - \frac{v^2}{c^2}}{c^2}} \]

Now squaring both sides

\[ m_2 = \frac{m_0^2}{\frac{1 - \frac{v^2}{c^2}}{c^2}} \]
\[ \frac{1 - \frac{v^2}{c^2}}{\frac{m_0^2}{m^2}} = \frac{\frac{v^2}{c^2}}{1 - \frac{m_0^2}{m^2}} = \frac{\frac{m^2 - m_0^2}{m^2}}{\frac{m^2 - m_0^2}{m^2}} = \frac{m^2}{c^2} \cdot \frac{m_0^2}{m^2} \]

\[ V_B = m^2 v^2 = c^2 (m^2 - m_0) \]

\[ \therefore \text{eqn } (3) \text{ becomes, } \]

\[ d = \frac{k}{\sqrt{c^2 (m^2 - m_0)}} \]

Multiplying and dividing by \( c \),

\[ d = \frac{k c}{\sqrt{c^4 (m^2 - m_0)}} \]

\[ \left[ \frac{E}{k} = c^2 (m - m_0) \right] \]

\[ L = \frac{k c}{\sqrt{c^2 (m - m_0) c^2 (m + m_0)}} \]

\[ \therefore d = \frac{k c}{\sqrt{K \left\{ c^2 (m - m_0 + 2m_0) \right\}} } \]

\[ = \frac{k c}{\sqrt{K \left\{ K + 2m_0c^2 \right\}} } \quad \text{Hence proved.} \]

Show that when e⁻ are accelerated through potential difference \( V \), their wavelengths taking relativistic character into account.
\[ d = \frac{h}{\sqrt{a^2 \varepsilon V m_0}} \left( \frac{1 - eV}{m_0 c^2} \right) \]

**Relative energy**

\[ E_k = c^2 \left[ \frac{m_0 - m_0}{\sqrt{1 - \frac{v^2}{c^2}}} \right] \]

\[ = m_0 c^2 \left[ \sqrt{1 - \frac{1}{1 - \frac{v^2}{c^2}}} - 1 \right] \]

\[ = m_0 c^2 \left[ \left( \frac{1 - \frac{v^2}{c^2}}{c^2} \right)^{-1/2} - 1 \right] \]

\[ = m_0 c^2 \left[ \frac{x + \frac{v^2}{2c^2}}{2c^2} - x \right] \]

\[ E_k = \frac{1}{2} m_0 v^2 \quad \text{directly with this} \]

**Proof**

\[ d = \frac{h}{m v} \]

\[ = \frac{h}{m_0 v} \]

\[ = \frac{h}{m_0 v} \left[ \sqrt{1 - \frac{v^2}{c^2}} \right]^{1/2} \]

\[ = \frac{h}{m_0 v} \left[ \frac{1 - \frac{v^2}{c^2}}{c^2} \right]^{1/2} \]

\[ = \frac{h}{m_0 v} \left[ \frac{1 - \frac{v^2}{c^2}}{c^2} \right]^{1/2} \]

\[ = \frac{h}{m_0 v} \left[ \frac{1 - \frac{v^2}{c^2}}{c^2} \right]^{1/2} - \left( \frac{1}{2} m_0 v^2 \right) \]

\[ E_k = eU = \frac{1}{2} m_0 v^2 \]
\[ v > \sqrt{\frac{2ev}{m_0}} \]

Putting this value in eqn (c)

\[ \frac{h}{\sqrt{2} ev m_0} \left( 1 - \frac{eV}{m_0 c^2} \right) \quad \text{then proved} \]

Our show that phase velocity of de-broglie waves associated with a moving particle having rest mass \( m_0 \) is given by

\[ v_p = c \sqrt{1 + \frac{m_0 c^2}{E^2}} \]

\[ \frac{1}{m_0} \frac{d}{dt} \left( \frac{mv}{\sqrt{1 - \frac{v^2}{c^2}}} \right) \]

\[ = \frac{h}{m_0 v} \left( \sqrt{1 - \frac{v^2}{c^2}} \right)^{-1} \]

\[ \Rightarrow \quad \frac{\sqrt{1 - \frac{v^2}{c^2}}}{m_0 v} = \frac{h}{m_0 v} \left( \sqrt{1 - \frac{v^2}{c^2}} \right)^{-1} \]

\[ \Rightarrow \quad \frac{\sqrt{1 - \frac{v^2}{c^2}}}{m_0 v} \left( \frac{h}{m_0 v} \right) \left( \sqrt{1 - \frac{v^2}{c^2}} \right)^{-1} = 1 \]

\[ \Rightarrow \quad \sqrt{1 - \frac{v^2}{c^2}} = \frac{c}{v} \]

Putting value of \( v^2 \) in \( \frac{1}{\sqrt{v^2 - c^2}} \)

\[ \frac{\sqrt{c^4 - \frac{c^2}{v^2}}}{m_0} \]

\[ \Rightarrow \quad v^2 = \frac{c^2}{v} \]

\[ \Rightarrow \quad v_p = \frac{c^2}{v} \]
\[ a = \frac{1}{m_e c^2} \int \frac{v_p^2}{c^2} - 1 \]

\[ m_e c^2 = \frac{1}{\hbar} \int \frac{v_p^2}{c^2} - 1 \]

Or, \[ \frac{v_p^2}{c^2} - 1 = \left( \frac{m_e c^2}{\hbar} \right)^2 \]

Or \[ v_p = \sqrt{1 + \left( \frac{m_e c^2}{\hbar} \right)^2} \]

two particles A and B are in motion if the wavelength associated with particle A is \( 5 \times 10^{-8} \text{ m} \). Calculate the wavelength of the particle B if its momentum is \( \frac{1}{2} \) that of \( A \).

\[ A_A = \frac{h}{p_A} \]

\[ A_B = \frac{h}{p_B} = \frac{h}{p_A} = \frac{2h}{p_A} \]

\[ = 2 \left( \frac{h}{p_A} \right) \]

\[ = 10^{-3} \text{ m} \]

Show that wavelength of 1500 m is not the correct wavelength for the particle if it is moving with velocity 600 m/s. How to be determined?
The energy of a particle at absolute temperature $T$ is of order of $k_B T$. Calculate wavelength of thermal neutrons at 27°C.

Given mass of deuterium = $m_D = 1.67 \times 10^{-27}$ kg

$$k_B = 1.38 \times 10^{-23} \text{ J} / \text{K}$$

**Sol.**

$$\lambda = h \frac{c}{2m_D T} \sqrt{\frac{2m_D k_B T}{\hbar^2}}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times 1.38 \times 10^{-23} \times 302}}$$
Heisenberg Uncertainty Principle.

The simultaneous determination of exact position and momentum of small moving particles is impossible.

\[ \Delta x \cdot \Delta p \geq \frac{\hbar}{2\pi} \]

or, \[ \Delta x \cdot \Delta p \geq \frac{\hbar}{4\pi} \]

or, \[ \Delta x \cdot \Delta p \approx \frac{\hbar}{2} \]

\( \Delta x \) = uncertainty in position of particle
\( \Delta p \) = uncertainty in momentum.

\[ \Delta E \cdot \Delta t \geq \frac{\hbar}{4\pi} \]

\[ \geq \frac{\hbar}{2} \]

\( \Delta E \) = uncertainty in energy of particle
\( \Delta t \) = "Time"

Application of Uncertainty Principle

1) Electrons do not exist inside the nucleus.

Proof: Let us assume e- exist inside the nucleus.
Nuclear radius \( r = 1 \times 10^{-15} \) m = 1 fm

2. \( A_x = \text{diameter of nucleus} \)
   \[ A_x = 2 \times 10^{-15} \text{m} \]

\[ A_P = \frac{\hbar}{A_x} \]

\[ = \frac{6.63 \times 10^{-34}}{2 \times 10^{-15}} \]

\[ = 3.31 \times 10^{-19} \text{ Kg m/s} \]

\[ E = \sqrt{P^2 c^2 + m^2 c^4} \]

\[ E = \sqrt{(3.31 \times 10^{-19})^2 (3 \times 10^8)^2 + (9.11 \times 10^{-31})^2 (3 \times 10^8)^4} \]

\[ E = 62 \text{ MeV} \]

Hence for the e\(^-\) to reside inside the nucleus, 62 MeV energy is needed. However, during \( \beta^- \) decay process, it was proved that for the e\(^-\) to reside inside the nucleus, \( 9 \text{MeV} \) energy is needed, which varies widely from our calculated result. Hence, our initial assumption is wrong. Therefore, e\(^-\) cannot exist inside the nucleus.

- Spectral lines have finite width.
- Schrödinger Time-independent Eqn.

General differential equation of wave is
\[ \frac{\partial^2 \psi}{\partial t^2} + \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\frac{\partial^2 \psi}{\partial z^2} - \frac{\partial^2 \psi}{\partial v^2} \]

where \( u = \) phase velocity.

\( \psi = \) wave function.

Solution of eqn (1) is of form:

\[ \psi = \phi \exp(-i\omega t) \]

\[ \frac{\partial \psi}{\partial t} = -i\omega \phi \exp(-i\omega t) \]

\[ \frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \phi \exp(-i\omega t) = -\omega^2 \psi - \phi \]

Put this in eqn (1)

Eqn (1) may be written as

\[ \nabla^2 \psi + \frac{\omega^2}{c^2} \psi = 0 \]

\[ \nabla^2 \psi + k^2 \psi = 0 \]

\[ k^2 = \frac{\omega^2}{c^2} = \frac{\pi^2}{a^2} \left( \frac{p}{a} \right)^2 \]

\[ a^2 = \frac{h^2}{\alpha} \]

Putting in eqn (1)

\[ \nabla^2 \psi + \frac{p^2}{\alpha^2} \psi = 0 \]
\[ E = k + V \]
\[ k = E - V \]
\[ p^2 = E - V \]
\[ \rho^2 = 2m(E - V) \]

Putting in eqn 4:

\[ \nabla^2 \psi + 2m(E - V)\psi = 0 \]

\[ \alpha^2 \]

**Time independent SWE**

For free particle:

\[ V = 0 \]

\[ \nabla^2 \psi + 2mE \psi = 0 \]

\[ \alpha^2 \]

**SWE for free particle**

**Time dependent SWE**

\[ \psi = \psi_0 e^{-i\omega t} \]

\[ \frac{\partial \psi}{\partial t} = -i\omega \psi_0 e^{-i\omega t} \]

\[ = -i\omega \psi \]

\[ = -i\varepsilon \pi^2 \psi \]

\[ = -i\frac{\omega}{\hbar} \psi \]

\[ = i\frac{E}{\hbar} \psi \]
\[ E\psi = \frac{-\hbar^2}{2m} \nabla^2 \psi + V \psi \]

where \( H = \frac{-\hbar^2}{2m} \nabla^2 + V \) is the Hamiltonian operator.
Orthogonality and normalization of wave functions:

\[ \int \psi^* \psi \, d\tau = 1 \quad \text{(normalized)} \]

\[ \int \psi^* \psi \, d\tau = 0 \quad \text{(orthogonal)} \]

If \( \psi = \sin \pi x \), then \( d\tau = dx \)

\[ \psi^* = \sin \pi x \]

\[ \psi = e^{i\theta} \]

\[ \psi^* = e^{-i\theta} \quad d\tau = dp \]

Thus find \( \psi = e^{ikx} \) as an acceptable ideal function, where \( k \) is some finite constant. Range: \(-\pi \leq x \leq \pi\)

Also normalize it given case.

Physical interpretation of wave function: Wave function \( \psi \) gives the behavior of particle at a particular position \( x \) and for given instant of time \( t \).

Its magnitude is large where the probability of finding the particle is high. However, it has a small magnitude where the probability of finding the particle is low. In other words...
We can regard $\psi$ as the probability of finding the particle at a given position.

Properties of wave function:
- Born postulate of $\psi$.
- It must be finite everywhere.
- It must be single valued.
- $\psi$ and its first derivative must be continuous everywhere.

Question: $\psi = \sin t$ is $0 < t < \frac{\pi}{2}$

$$\frac{d\psi}{dt} = \cos t$$

Solve:
$$\psi = e^{ikx}$$

$$\frac{d\psi}{dz} = ike^{ikx}$$

Using Normalization criterion:
$$\frac{1}{\sqrt{2\pi}} \int\psi \overline{\psi} dx = 1$$

Let $\psi = A e^{ikx}$

$$\overline{\psi} = A^* e^{-ikx}$$

$$\int A^* e^{-ikx} A e^{ikx} dx = 1$$

$$\int |A|^2 dx = 1$$

$$|A|^2 \left[ x^2 \right]_0^\infty = 1$$

$$\int |A|^2 dx = 1$$
cor. \[ A = \frac{\sqrt{2a}}{L} \]

As normalise the wave function:
\[ \psi = \frac{\sin \pi x}{L} \quad 0 < x < L \]

Let \[ \psi = \frac{A \sin \pi x}{L} \]

\[ \psi^* = \frac{A \sin \pi x}{L} \]

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

\[ \int_{-a}^{a} A^2 \sin^2 \frac{n \pi x}{L} \, dx = 1 \]

\[ |A|^2 \int_{0}^{L} \sin^2 \frac{n \pi x}{L} \, dx = 1 \]

\[ |A|^2 \left[ \frac{L - \cos \frac{2n \pi x}{L}}{2} \right]_{0}^{L} = 1 \]

\[ \cos \left( \frac{2 \pi x}{L} \right) \bigg|_{0}^{L} = 0 \]

\[ \int_{0}^{L} x - \frac{\sin \frac{2 \pi x}{L}}{2} \bigg|_{0}^{L} = 1 \]

\[ \int_{0}^{L} \psi^* \psi \, dx = 1 \]

\[ \int_{-a}^{a} A^2 \sin^2 \frac{n \pi x}{L} \, dx = 1 \]

\[ \int_{-a}^{a} A^2 \sin^2 \frac{n \pi x}{L} \, dx = 1 \]

\[ |A|^2 \int_{0}^{L} \psi^2 \, dx = 1 \]

\[ |A|^2 \left[ \frac{L}{2} \right] = 1 \]

\[ |A|^{2} = \frac{2}{L} \]

\[ A = \frac{\sqrt{2}}{L} \quad \psi = \frac{\sqrt{2} \sin \pi x}{L} \]
Operators

1. Position operator \( \hat{x}, \hat{y}, \hat{z} \)
2. Energy operator \( \hat{E} = \hat{P}^2 + \frac{\hat{V}}{2m} \)
3. Hamiltonian operator \( \hat{H} = \hat{P}^2 + \frac{\hat{V}}{2m} \)
4. Momentum operator \( \hat{p} = p = \frac{\hbar}{i} \partial_x \phi \)

\[ \phi = \phi_0 \, e^{-\frac{i}{\hbar} (\omega t - kx)} \]
\[ \phi = \phi_0 \, e^{-\frac{i}{\hbar} \sqrt{\frac{\hbar}{m} E - E}} \]
\[ \phi = \phi_0 \, e^{-\frac{i}{\hbar} \sqrt{\frac{\hbar}{m} E}} \]
\[ \phi = \phi_0 \, e^{-\frac{i}{\hbar} \sqrt{\frac{\hbar}{m} E}} \]
\[ \phi = \phi_0 \, e^{-\frac{i}{\hbar} \sqrt{\frac{\hbar}{m} E}} \]

\[ \frac{\partial \psi}{\partial x} = -i \hbar \frac{\partial \psi}{\partial t} \]
\[ \sigma_x \psi = i \hbar \frac{\partial \psi}{\partial t} \]
\[ \phi = \tan \left( \frac{i \hbar}{\partial \psi} \right) \]

Multiply on the inside by \( i \)
\[ \hat{y} = -i \hbar \frac{\partial}{\partial y} \]
\[ \hat{p}_z = -i \hbar \frac{\partial}{\partial z} \]
\[ \hat{p} = -i \hbar \hat{\nabla} \]

We write down the position, energy, Hamiltonian, and momentum operators and don't derive the operators.

**Expectation values of operators**

\[ \langle x \rangle = \int \psi^* x \psi \, d\tau \]
\[ \langle y \rangle = \int \psi^* y \psi \, d\tau \]
\[ \langle E \rangle = \int \psi^* \hat{E} \psi \, d\tau \]

\[ \hat{E} = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial \tau^2} \]

\[ = \int \psi^* \left( \frac{\hbar^2}{2m} \frac{\partial^2}{\partial \tau^2} \right) \psi \, d\tau \]
\[ = \frac{i\hbar}{\hbar} \int \psi^* \frac{\partial^2}{\partial \tau^2} \psi \, d\tau \]
\[ = \frac{i\hbar}{\hbar} \int \psi^* \frac{\partial}{\partial \tau} \left( \frac{\partial}{\partial \tau} \right) \psi \, d\tau \]

\[ \langle \hat{p}_x \rangle = \int \psi^* \hat{p}_x \psi \, d\tau \]
\[ = \int \psi^* \left( -i \hbar \frac{\partial}{\partial x} \right) \psi \, d\tau \]
\[ = - \int \psi^* \left( -i \hbar \frac{\partial}{\partial x} \right) \psi \, d\tau \]
\[ = -i \hbar \int \psi^* \frac{\partial}{\partial x} \psi \, d\tau \]
Find the expectation value of $\hat{p}$ for the wave function $\psi = \frac{1}{\sqrt{L}} \sin \frac{\pi x}{L}$ for $0 < x < L$.

$$\langle \hat{p} \rangle = \int x \psi^* \hat{p} \psi \, dx$$

$$= \int \frac{1}{\sqrt{L}} \sin \frac{\pi x}{L} \left(-i \hbar \frac{\partial}{\partial x} \right) \left( \frac{1}{\sqrt{L}} \sin \frac{\pi x}{L} \right) \, dx$$

$$= -i \frac{\hbar}{L} \int \sin \frac{\pi x}{L} \frac{\partial}{\partial x} \sin \frac{\pi x}{L} \, dx$$

$$= -i \frac{\hbar}{L} \int \frac{\pi}{L} \cos \frac{\pi x}{L} \sin \frac{\pi x}{L} \, dx$$

$$= -i \frac{\hbar \pi}{L^2} \int \frac{\pi}{L} \sin^2 \frac{\pi x}{L} \, dx$$

$$= -i \frac{\hbar \pi}{L^2} \left[ \frac{x}{2} - \frac{\sin 2\pi x}{4\pi} \right]_0^L$$

$$= -i \frac{\hbar \pi}{L^2} \left[ \frac{L}{2} - 0 \right]$$

$$= -i \frac{\hbar \pi L}{2L^2}$$

$$= -i \frac{\hbar \pi}{2L}$$
\[ \langle p^2 \rangle = \int \frac{p^4}{2m} (\frac{\sigma x}{L})^2 \frac{1}{L} \sin^2 \frac{\sigma x}{L} \, dx \]

\[ = \int \frac{1}{2} \sin^2 \frac{\sigma x}{L} \left( -\frac{i \hbar \sigma}{L} \right)^2 \left( \frac{\sigma^2 x^2}{L^2} \right) \, dx \]

\[ = -\frac{\hbar^2 \sigma^2}{2L^2} \int \frac{\sin^2 \frac{\sigma x}{L}}{L^2} \frac{d^2}{dx^2} \sin^2 \frac{\sigma x}{L} \, dx \]

\[ = -\frac{\hbar^2 \sigma^2}{L^2} \int \frac{\sin^2 \frac{\sigma x}{L}}{L^2} \frac{d^2}{dx^2} \sin^2 \frac{\sigma x}{L} \, dx \]

\[ = \frac{\sigma^2 \hbar^2}{L^2} \int \frac{d^2}{dx^2} \left( 1 - \cos^2 \frac{\sigma x}{L} \right) \, dx \]

\[ = \frac{\pi^2 \hbar^2}{L^2} \int \left[ \frac{d}{dx} - \frac{L}{\sigma} \sin \frac{\sigma x}{L} \right] \, dx \]

\[ = \frac{\pi^2 \hbar^2}{L^2} \left[ \frac{L}{\sigma} \sin \frac{\sigma x}{L} \right]_0^\pi \]

\[ = \frac{\pi^2 \hbar^2}{L^2} \left( \frac{L}{\sigma} \right) \]

\[ = \frac{\pi^2 \hbar^2}{L} \frac{L}{\sigma} \]

\[ = \frac{\pi^2 \hbar^2}{\sigma} \]

Why find the expectation value of energy for the wave function:

\[ \psi = \frac{1}{L} \sin \frac{\sigma x}{L} \quad \text{for } 0 \leq x \leq L \]

SOL:

\[ \langle E \rangle = \langle \frac{\hbar^2}{2m} \rangle \]

\[ = \langle p^2 \rangle \frac{L^2}{2} \frac{\sigma^2}{L^2} \]

\[ = \langle p^2 \rangle \frac{\sigma^2}{2} \]

\[ \langle \frac{\sigma^2}{2} \rangle = \frac{\pi^2 \hbar^2}{2m L^2} \]
Particle in one dimensional box or square well potential.

\[ v(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{for } x < 0, x > L \end{cases} \]

In region I, i.e. inside well, SWE is

\[ \frac{d^2 \psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0. \]

Cor. \[ \frac{d^2 \psi}{dx^2} + \alpha^2 \psi = 0 \quad (\alpha^2 = \frac{2mE}{\hbar^2}) \]

Let \( \psi \) of eq. (2) be

\[ \psi = Ae^{i\alpha x} + Be^{-i\alpha x} \quad (3) \]

Boundary conditions:

1. At \( x = 0 \), \( \psi = 0 \)
2. At \( x = L \), \( \psi = 0 \)
Applying $\phi$ in (3)

$$A + B x e^{i \theta}$$

$$B = -A$$

\[ \therefore \text{eq (3) may be written as,} \]

$$\phi = A e^{-i \alpha x}$$

$$= A \left[ e^{i \alpha x} - e^{-i \alpha x} \right]$$

\[ \therefore \phi = A \left[ \cos \alpha x + i \sin \alpha x - \cos \alpha x - i \sin \alpha x \right] \]

or, \[ \phi = A \left[ \cos \alpha x + \sin \alpha x \right] \]

\[ \phi = A' \sin \alpha x \]

(6) where $A' = 2iA$

Apply boundary eqn in eqn (6)

\[ D = A' \sin \alpha x L \]

\[ \therefore \sin \alpha x L = 0 \]

\[ \alpha x L = n \pi \quad (n = 0, 1, 2, \ldots) \]

\[ 0 < x = \frac{n \pi}{L} \]

\[ \therefore \text{eq (6) will become,} \]

$$\phi = A \sin \frac{n \pi x}{L}$$

(7)

Energy Eigen Value,

from (3) and (7)

$$\sqrt{\frac{2m}{\hbar^2}} = \frac{n \pi}{L}$$

or,

$$E = \hbar^2 \frac{n^2 \pi^2}{L^2} \frac{\pi^2}{2mL^2}$$

(8) \[ (n = 1, 2, 3, \ldots) \]
\[ E = \frac{n^2 \hbar^2}{8mL^2} \]

Set \( n \to \infty \),

\[ K = \frac{\hbar^2}{2m} \]

\( \left( n = 1, 2, 3, \ldots \right) \)

Significance of zero point energy

Here \( n \to \infty \) because at \( n = 0 \) the wave function of the particle becomes zero \( (\psi = 0) \) which means the particle is not present at all. This contradicts our initial assumption that at least one particle is present inside the box.

\( n \to 0 \) also means that the particle can have zero energy; hence, the lowest possible energy \( 0 \) for the state energy, which the particle can have, will be \( n = 1 \).

At \( n = 1 \),

\[ E_1 = \frac{\hbar^2}{8mL^2} \]

\[ E_2 = \frac{3\hbar^2}{8mL^2} \]

At \( n = 2 \),

\[ E_2 = \frac{\hbar^2}{8mL^2} \]

\[ E_3 = \frac{9\hbar^2}{8mL^2} \]

At \( n = 3 \),

\[ E_3 = \frac{9\hbar^2}{8mL^2} \]

\[ E_4 = \frac{25\hbar^2}{8mL^2} \]

Energy levels are not equally distributed.

Normalized wave function

\[ \int_{-\frac{L}{2}}^{\frac{L}{2}} y^2 dx = 1 \]
\[ \int_0^L \frac{A^2 \sin^2 \pi x}{2} \frac{1}{2} \sin^2 \pi x \, dx = 1 \]
\[ \int_0^L \frac{A^2}{2} \left( 1 - \cos 2 \pi x \right) \, dx = 1 \]
\[ \frac{1}{2} \left[ L - \frac{2 \pi}{L} \sin 2 \pi x \right]_0^L = 1 \]
\[ \frac{1}{2} \left[ \frac{2 \pi}{L} \right] = \frac{1}{2} \]
\[ A^2 = \frac{2}{L} \]
\[ A = \sqrt{\frac{2}{L}} \]

Hence normalized wave function
\[ \psi = \sqrt{\frac{2}{L}} \sin \pi x \]

Eqn. (1) represents the normalized wave function of the particle trapped in a one-dimensional box of length \( L \).

\( n = 1 \), \( \psi = 0 \) at \( x = 0 \)
\( n = 1 \), \( \psi = 0 \) at \( x = L \) and \( x = 0 \)
\( n = 2 \), \( \psi = 0 \) at \( x = 0 \), \( n > 2 \) and \( \psi = 0 \)
\( n = 3 \), \( \psi = 0 \) at \( x = 0 \), \( x = L \) and \( x = \frac{L}{3} \)
At \( n=1 \) 1 two nodes are present at \( x=0 \) and \( x=L \)

At \( n=2 \) 2 nodes are present at \( x=L/2 \)

At \( n=3 \) 4 nodes are present at \( x=0 \)

Hence we conclude that there are \( n+1 \) nodes for each value of \( n \).

\[ \psi_n = \begin{cases} 
\text{for } n=0 & \psi_0 = 1 \\
\text{for } n=1 & \psi_1 = \sin \frac{\pi x}{L} \\
\text{for } n=2 & \psi_2 = 2 \sin \frac{2\pi x}{L} \\
\text{for } n=3 & \psi_3 = 4 \sin \frac{3\pi x}{L} \\
& \vdots 
\end{cases} \]

Probability \( P = \frac{1}{L} \int_0^L |\psi|^2 \, dx \)

\[ P = \frac{2}{L} \sin^2 \frac{n \pi x}{L} + \frac{1}{L} \]

Probability max when

\[ \frac{n \pi x}{L} = \frac{2\pi}{2}, \frac{4\pi}{2}, \frac{6\pi}{2}, \ldots \]
\[ x = \frac{L}{2n^2} \]

**Step potential**

\[ V(x) = \begin{cases} V_0 & \text{for } x > 0 \\ 0 & \text{for } x < 0 \end{cases} \]

\[ x = 0 \]

**Finite square well**

\[ V(x) = \begin{cases} V_0 & \text{for } x > 0 \\ 0 & \text{for } x < 0 \end{cases} \]

\[ x = 0 \]

**Potential Barrier**

\[ V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x > 0 \end{cases} \]

\[ x = 0 \]

**Schrödinger wave eqn in region I**

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_1 + V_1 \psi_1 = E \psi_1 \]

\[ \psi_1(0) = 0, \quad \frac{d\psi_1}{dx}(0) = 0 \]

**Schwarzschild**

\[ \frac{d^2}{dx^2} \psi_2 + \frac{2m}{\hbar^2} \left( (E - V_0) \psi_2 \right) = 0 \]

\[ \frac{d^2}{dx^2} \psi_2 + \frac{p_1^2}{\hbar^2} \psi_2 = 0 \]

where, \( p_1^2 = 2mE \)
where \[ p_z = 2m(E-V_0) \]

So if eqn (1) and (2) is

\[ \psi = A e^{ip_zx/\hbar} + Be^{-ip_zx/\hbar} \]

\[ \psi_2 = Ce^{i(p_z+\alpha)x/\hbar} + De^{-i(p_z+\alpha)x/\hbar} \]

In eqn (5) first term represents the wave travelling along the axis in region I and it represents the incident wave. The second term represents the wave travelling along \(-ve\) x-axis in region I and it represents the reflected wave.

In eqn (6) first term represents the wave travelling along the x-axis in region II and it represents the transmitted wave. Since region II is a continuous region, hence nothing is reflected back in the region II. Hence the second term of region II should not exist.

Hence the wave function of the particle in region II will be given by

\[ \psi_2 = Ce^{i(p_z+\alpha)x/\hbar} \]

Here A, B, C are constants which are determined by the boundary conditions.
Boundary condition,
\[ \psi_1 = \psi_2 \text{ at } x = 0 \]  \( \circ \)
\[ \frac{d \psi_1}{dx} = \frac{d \psi_2}{dx} \text{ at } x = 0 \]  \( \circ \)

Applying boundary condition \( \circ \) in eqn \( \circ \) and \( \circ \)
\[ A + B = C \]  \( \circ \)

\[ \frac{d \psi_1}{dx} = i \rho_1 \left[ A e^{i \rho_1 x} + B e^{-i \rho_1 x} \right] \]  \( \circ \)

\[ \frac{d \psi_2}{dx} = i \rho_2 C e^{i \rho_2 x} \]  \( \circ \)

Applying \( \circ \) in eqn \( \circ \) and \( \circ \),
\[ \frac{1}{i} \left[ A - B \right] = \frac{i \rho_1}{\rho_1} C. \]
\[ \text{for } A - B = \rho_2 C \]  \( \circ \)

Adding eqn \( \circ \) and \( \circ \)
\[ 2A = \left( 1 + \frac{\rho_2}{\rho_1} \right) C \]

Or,
\[ 2A = \left( \frac{\rho_1 + \rho_2}{\rho_1} \right) C \]

Or,
\[ \left( \frac{C}{A} \right) = \frac{2\rho_1}{\rho_1 + \rho_2} \]  \( \circ \)
Reflectance: \[ R = \frac{\text{magnitude of reflected wave}}{\text{incident wave}} \]

Transmittance: \[ T = \frac{\text{magnitude of transmitted wave}}{\text{incident wave}} \]

Case I: when \( E \geq V_0 \)

\[ P_2 = \text{real} \]

\[ R = \frac{|B|^2}{A} = \left( \frac{p_1 - p_2}{p_1 + p_2} \right)^2 \]

\[ T = \frac{|C|^2}{A} = \left( \frac{2p_1}{p_1 + p_2} \right)^2 \]

\[ R + T = 1 \]

When \( E = V_0 \),

\[ P_2 = 0 \]

\[ R = 1 \]

\[ T = 0 \]

\[ \frac{\text{probability current density}}{S_x} \]

\[ \frac{1}{2\pi m} \int \frac{r_y - rf_1}{dx} \]
\[ \psi_1 = A e^{ip_1x/\hbar} + B e^{-ip_1x/\hbar} \]

\[ \psi_1^* = A^* e^{ip_1x/\hbar} + B^* e^{-ip_1x/\hbar} \]

\[ \frac{d \psi_1}{dx} = \frac{ip_1}{\hbar} \left[ A e^{ip_1x/\hbar} - B e^{-ip_1x/\hbar} \right] \]

\[ \frac{d \psi_1^*}{dx} = -\frac{ip_1}{\hbar} \left[ A^* e^{-ip_1x/\hbar} - B^* e^{ip_1x/\hbar} \right] \]

\[ \frac{1}{2im} \left[ 2im \left( A e^{-ip_1x/\hbar} + B e^{-ip_1x/\hbar} \right) \frac{d \psi_1}{dx} - \left( A^* e^{ip_1x/\hbar} - B^* e^{-ip_1x/\hbar} \right) \psi_1^* \right] \]

\[ (S_x) = \frac{1}{2im} \left[ A^* A + B A^* e^{ip_1x/\hbar} - A B^* e^{-ip_1x/\hbar} - B^* A \right] \]

\[ = \frac{p_1^2}{2m} \left[ A^2/2^2 - 2 |B|^2 \right] \]

\[ = \frac{p^2}{2m} \left[ |A|^2 - |B|^2 \right] \]

\[ (S_x)_I = \frac{k}{2im} \left[ \psi_1^* \frac{d \psi_1}{dx} - \frac{d \psi_1^*}{dx} \psi_1 \right] \]
\[ \psi_2 = C e^{i p_2 x / \hbar} \]

\[ \psi_2^* = C^* e^{-i p_2 x / \hbar} \]

\[ \frac{d}{dx} \psi_2 = \frac{i p_2}{\hbar} C e^{i p_2 x / \hbar} \]

\[ \frac{d}{dx} \psi_2^* = -\frac{i p_2}{\hbar} C^* e^{-i p_2 x / \hbar} \]

\[ (S_x)_D = \frac{1}{2m} \int \left( C e^{-i p_2 x / \hbar} \right) \frac{i p_2}{\hbar} C e^{i p_2 x / \hbar} \right) - \frac{C C^* e^{-i p_2 x / \hbar}}{\hbar} \]

\[ (S_x)_D = \frac{p_2}{2m} \left[ 2 \text{Im} \right] \]

\[ (S_y)_D = \frac{p_2}{2m} \left| C \right|^2 \]

\[ R = \frac{\pi/m}{\sqrt{\left| B \right|^2}} = \frac{1}{\sqrt{\left| A \right|^2}} = \frac{\left| B \right|^2}{\left| A \right|^2} = \frac{\left| B \right|^2}{\left| A \right|^2} \]

\[ T = \frac{\left| p_2 / m \right|}{\sqrt{\left| A \right|^2}} \left| C \right|^2 = \frac{p_2}{\left| p_1 \right|} \left( \frac{C}{A} \right)^2 \]

\[ T = \frac{p_2 \cdot \left| C \right|^2}{\left| A \right|^2} \frac{\left| p_1 \right|^2}{\left| p_1 + p_2 \right|^2} \frac{\left| A \right|^2}{\left| A \right|^2} \]
Case I. when $E = V_0$

$$p_2 = \sqrt{2m(E-V_0)} = 0$$

$\frac{1}{m} T = 0$

$\frac{1}{m} R = 1$

Case II. when $E < V_0$

$p_2 = \sqrt{2m(E-V_0)}$

$$= \sqrt{2m(V_0-E)}$$

$$= i\sqrt{2m(V_0-E)}$$

$p_2^* = -i\sqrt{2m(V_0-E)} = -p_2$

$$(\mathbf{S}_x)_2 = \frac{1}{2im} \left( \psi_2^* \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_2^*}{dx} \right)$$

$\psi_2 = Ce^{ip_2 x / \hbar}$

$\psi_2^* = C e^{-ip_2^* x / \hbar} = C e^{ip_2 x / \hbar}$

$$\frac{d\psi_2}{dx} = \frac{ip_2}{\hbar} Ce^{ip_2 x / \hbar}$$

$$\frac{d\psi_2^*}{dx} = \frac{ip_2^*}{\hbar} Ce^{-ip_2 x / \hbar}$$
\[
B = 1 - \int \left( e^{-i2\pi x/t} + e^{i2\pi x/t} \right) dx \quad \text{for} \quad \text{constant} \quad \alpha
\]
Cubic crystals

(i) Simple cubic

In this there are one lattice point per unit cell. A lattice point is situated at the corners of the cube. A unit cell containing only one lattice point is called a primitive cell. Therefore, simple cubic lattice is also called primitive-lattice.

Coordination no. \(2 \times 6 = 12\)

\[ \pm a, \pm a, \pm a \]

\[ (\pm a, 0, 0), (0, \pm a, 0), (0, 0, \pm a) \]

\[ (a, a, 0), (-a, -a, 0) \]

\[ (0, a, a), (a, 0, -a) \]

\[ (0, 0, a), (a, -a, a) \]

Distance between nearest neighbours

\[ \sqrt{a^2 + a^2 + a^2} = a \text{ (lattice constant)} \]

(ii) Body centered cubic

\[ \frac{z}{2} \]
There is one lattice point at each corner of the cube, and one lattice point is situated at the center of the body. Each cell has 8 corners and 8 cells meet at each corner. Therefore, each lattice point at corner belongs to one unit cell. Also, there is one lattice point at center of the body, therefore total no. of lattice point in any one cell is \((8 \times 1) + 1 = 2\).

Hence, there are 2 lattice points per unit cell.

Coordination no.

\[
\left( \pm \frac{a}{2}, \pm \frac{a}{2}, \pm \frac{a}{2} \right)
\]

\[
\left( \frac{a}{2}, \frac{a}{2}, \frac{a}{2} \right) \left( \frac{a}{2}, \frac{a}{2}, \frac{a}{2} \right)
\]

\[
\left( \frac{a}{2}, -\frac{a}{2}, -\frac{a}{2} \right) \left( -\frac{a}{2}, \frac{a}{2}, -\frac{a}{2} \right) \left( \frac{a}{2}, -\frac{a}{2}, \frac{a}{2} \right)
\]

\[
\left( -\frac{a}{2}, -\frac{a}{2}, \frac{a}{2} \right) \left( \frac{a}{2}, -\frac{a}{2}, \frac{a}{2} \right)
\]

Distance b/w nearest neighbors

\[
\sqrt{\left( \frac{a}{2} \right)^2 + (9)^2 + \left( \frac{a}{2} \right)^2} = \sqrt{\frac{a^2}{4} + 81 + \frac{a^2}{4}} = \sqrt{\frac{82a^2}{4}} = \frac{\sqrt{82}a}{2}
\]
In this there is one lattice point at each corner of the cube and one lattice point at each face of the cube. Each unit cell has 8 corners and 6 cells meet at each corner. Therefore, \( \frac{1}{8} \) of a lattice point at each corner belongs to any one cell.

Also, there is one lattice point at the center of each face of the cell and it is shared by two cells. Therefore, only \( \frac{1}{2} \) of a lattice point belongs to any one cell. Since a cell has 8 corners and 6 faces, therefore, total no. of lattice points is \( \left( \frac{1}{8} \times 8 \right) + \left( \frac{1}{2} \times 6 \right) = 4 \)

Coordination no.: 12

- \( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \)
- \( \frac{1}{2}, \frac{1}{2}, 0 \)
- \( 0, \frac{1}{2}, \frac{1}{2} \)
- \( \frac{1}{2}, 0, \frac{1}{2} \)
- \( 0, \frac{1}{2}, 0 \)
- \( \frac{1}{2}, 0, 0 \)
- \( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \)
- \( 0, \frac{1}{2}, \frac{1}{2} \)
- \( \frac{1}{2}, 0, \frac{1}{2} \)
- \(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \)
- \( \frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \)
- \( -\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \)
\[(0, 0, 1) (0, 1, 0) (1, 0, 0)\]

Distance to nearest neighbours:

\[\sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{1}{2}\right)^2} = \frac{a}{\sqrt{2}}\]

\[J = \frac{a}{\sqrt{2}}\]

Derive the lattice constant \(a\) as

\[a = \left(\frac{\rho M}{N}\right)^{1/3}\]

\(\rho = \text{no. of mol} \text{ per unit volume}\)

\(M = \text{mol. wt.}\)

\(N = \text{Avagadro no.}\)

\(\rho = \text{density}\)

\(a = \text{lattice constant}\)

\(\frac{V_0}{N} = a^3\)

\[\rho = \frac{m}{a^3}\]

\[m = \frac{N M}{N}\]

\[\rho = \frac{m}{N a^3}\]

\[a^3 = \left(\frac{N M}{\rho N}\right)^{1/3}\]
Miller Indices

Position and orientation of a lattice plane in a crystal is determined by smallest whole number ratios with one another as reciprocal of intercept of the plane on three crystal axes. These are denoted by $h, k, l$ and are called as Miller Indices.

The direction of other face of the crystal is governed by law of rational indices. This law states that a plane which is parallel to a plane whose intercepts on the three axes are $m_1, a, m_2, b, m_3, c$ where $m_1, m_2,$ and $m_3$ are smallest whole no. is the possible face of the crystal.
If $a', b', c'$ are the possible face edges of a crystal, then $DA \cdot OB \cdot OC = \frac{m_1}{m_2} \cdot \frac{m_2}{m_3}$

$$= \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$$

where $h = m_2 m_3$

$k = m_1 m_3$

$l = m_1 m_2$

Our final Miller indices of a crystal are the three axes are

$2a : 3b : 4c$

$$2a + 3b + 4c = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$$

$h : k : l = 1 : 1 : 1$

$$\frac{2}{3} \cdot \frac{3}{4} \cdot \frac{4}{3}$$

$(h, k, l) = (643)$

Deducing Miller indices of plane in an orthorhombic crystal, which contains

$2a, -2b, \frac{2c}{2}$

$$3a : -2b : 2c = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$$
An orthorhombic crystal has axial ratios in the ratio $0.424:1:0.362$. The Miller indices whose intercepts are in the ratio $0.362:1:0.183$ are $\{h, k, l\}$. Sketching of lattice planes:

- $(1, 0, 0)$
- $(0, 1, 0)$
- $(0, 0, 1)$
- $(1, 1, 0)$
Interplanar Spacing

The separation between successive lattice planes of cubic, tetragonal and orthorhombic crystal, for which $a = b = c = 90^\circ$ is called interplanar spacing.

Let $OX$, $OY$ and $OZ$ are three axes parallel to crystal axes. Let $ABC$ be the plane of the crystal. Let $A$, $B$, $C$ be intercepts. $OA = b$, $OB = \frac{1}{2}$, $OC = \frac{1}{3}$.

Let $ON$ be the length of normal from origin to the plane $ABC$ and is equal to small $d$. Which is called...
In-interplanar spacing, let \( \theta_a, \theta_b, \theta_c \) are the angles which ON makes with the three axes.

Direction cosines of ON are,

\[
\cos \theta_a = \frac{ON}{OA}, \quad \cos \theta_b = \frac{ON}{OB}, \quad \cos \theta_c = \frac{ON}{OC}
\]

Also,

\[
\cos^2 \theta_a + \cos^2 \theta_b + \cos^2 \theta_c = 1
\]

\[
\left( \frac{ON}{OA} \right)^2 + \left( \frac{ON}{OB} \right)^2 + \left( \frac{ON}{OC} \right)^2 = 1
\]

\[
\frac{a^2}{h^2} + \frac{b^2}{k^2} + \frac{c^2}{l^2} = 1
\]

\[
g = \frac{1}{\sqrt{\frac{a^2}{h^2} + \frac{b^2}{k^2} + \frac{c^2}{l^2}}}
\]

\[
d = \frac{a}{\sqrt{a^2 + b^2 + c^2}}
\]

for cubic crystals, \( a = b = c \).

\[
d = \frac{a}{\sqrt{a^2 + b^2 + c^2}}
\]

Simple cubic,

\[
d_{100} = a
\]

\[
d_{110} = \frac{a}{\sqrt{2}}
\]

\[
d_{111} = \frac{a}{\sqrt{3}}
\]

\[
d_{100} \neq d_{110} \neq d_{111}
\]
Body centred

In BCC crystal there exist an additional plane halfway between 100 and 111.

\[ d_{100} = \frac{a}{2} \]
\[ d_{110} = \frac{a}{\sqrt{2}} \]
\[ d_{111} = \frac{a}{2 \sqrt{3}} \]

\[ d_{100} : d_{110} : d_{111} = \frac{1}{2} : \frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}} \]

Multiply numerator by 2:

\[ 1 : \frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}} \]

Face centred

In FCC crystals there exist an additional plane halfway between 100 and 110 plane.

\[ d_{100} = \frac{a}{2} \]
\[ d_{110} = \frac{a}{\sqrt{2}} \]
\[ d_{111} = \frac{a}{2 \sqrt{3}} \]

\[ d_{100} : d_{110} : d_{111} = \frac{1}{2} : \frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}} \]

Multiply by 2 in numerator:

\[ 1 : \frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}} \]
Bragg's Law

Diffractive of X-rays in crystal is called Bragg's Law.

Let an X-ray beam is incident on a crystal at point A. It started in random directions. 'd' is the smallest separation by the crystal. BC and BD are perpendicular to the reflected ray.

Path difference:

\[ BC + BD = a \sin \theta + d \sin \theta = 2a \sin \theta \]

For maxima, \[ 2a \sin \theta = n \] Bragg's Law

Laue's Experiment:

In Laue's method, a single crystal is held stationary in a continuous X-ray beam. The crystal diffracts the wavelength for which the crystal plane or spacing is the incidence.
angle and satisfies the Bragg's law. In Laue's experiment, a continuous x-ray beam is collimated by a pin-hole arrangement and allowed to fall on a crystal. A flat film is placed to receive transmitted and reflected beams. The dispersion may consists of a series of monochromatic Laue's pattern.

The distribution of spots in Laue's pattern depend upon the symmetry of crystal and its orientation with respect to x-ray beam.

Applying this method is convenient for rapid determination of crystal orientation. symmetry axis is succeeded in only three cases, as it is also known as the 3Crystalline imperfections were mechanical and thermal treatment.

In an crystal lattice there exists many planes with different orientation spacing with a common origin normal to all set of planes, the length of each normal being proportional to the reciprocal of the interplanar spacing. The end point on normal from lattice is called reciprocal lattice.
Module 11  Semiconductors and Superconductors

Semiconductors - free free e⁻, metals
Insulators - NO free e⁻, good plastic

Semiconductors - Si, Ge

Intrinsic  Extrinsic
(pure Semiconductor) Type N-type

Donor (Conduction)  Acceptors
Impurities (B, Al) (As, Antimony)

Classification of solids on basis of Band diagram

Conductors

C.B  v.B

Overlap of C.B, v.B

Insulators  C.B

\[ E_g = 3.5 \text{ eV} \]

\[ v_B \]

Intrinsic Semiconductors

C.B  \[ E_g = 1 \text{ eV} \]

v.B
In intrinsic semiconductors, the Fermi level lies exactly between the conduction band and the valence band.

In p-type semiconductors, the Fermi level lies just below the bottom of the CB.

In n-type semiconductors, the Fermi level lies just above the top of VB.
Superconductors

In 1911, Kamerlingh Onnes found that at very low temperatures the resistance of mercury first decreases with the decrease in temp., but at 4.2 K Kelvin the resistance suddenly returns to zero.

\[ T \]

- normal metals

The temp. at which this phase transition occurs is known as critical temperature or transition temperature.

Similar observations were made for aluminium, lead, tin, In, Zn. This phenomenon of electrical resistivity at a particular transition temperature is known as superconductivity, and the materials which follow this phenomenon are known as superconductors.

Properties of superconductors
1) At room temp. superconductors show higher resistivity than normal metals.

2) Transition temp. is different for different isotopes. It decreases with the increase in atomic weight. This is known as isotopic effect in superconductors.

3) When large magnetic field is applied in the superconductor, its superconducting property is destroyed.

4) The current in superconductor flows according to the relation

\[ \frac{\Delta I}{\Delta t} = \frac{I}{R} \]

\[ I = \frac{V}{R} \]

\[ L = \text{Time constant} \]

\[ R \rightarrow 0, \quad 1/R \rightarrow \infty \]

the current in superconductor flows for infinite period of time till the temperature remains constant. This current is called persistent current.

Meissner effect:

When a long superconductor is placed in magnetic field, below critical temperature, the magnetic lines of force are pushed out of the specimen of superconductor. This phenomenon is called the Meissner effect.
\( B_{\text{int}} = \mu_0 (H + M) \)

where \( \mu_0 \) = permeability of free space

\( \vec{H} = \) magnetic field intensity

\( \vec{M} = \) magnetic moment per unit volume

Here \( B_{\text{int}} = 0 \)

\( \mu_0 (H + \vec{M}) = 0 \)

or, \( \vec{H} = -\vec{M} \)

\( \chi = M / H \)

\[ \chi = -1 \]

Diamagnetic

Meissner effect is a kind of diamagnetism.

BCS Theory (Bardeen, Cooper and Schrieffer)

Explained that just like electrons with opposite spins form pairs, there is attractive interaction.
The e- and phonons and they form quasi-pairs. These quasi-pairs are called Cooper pairs.

Phonons are quanta of longitudinal sound waves.

Types of superconductors:

Type I and Type II superconductors

1) In Type I superconductors, superconductivity is abruptly destroyed when the intensity of applied magnetic field exceeds above a critical value. In Type II superconductors, when the magnetic field is increased above a critical value it leads to a mixed state in which an increasing amount of magnetic flux penetrates into the material, but there is no electric current inside the material.

2) Type I superconductors are also called 1st-generation. Type II are called 2nd-generation superconductors.

3) In Type I superconductors, the diamagnetic moment drops to zero and resistivity goes to its normal value. In Type II, without the diamagnetic moment start to decrease, but the resistivity does not return, this is called mixed state of Type II superconductors.
Density of states for free e⁻ (derivation)

\[ \psi = e^{i(k \cdot r - \omega t)} \]

SWE,

\[ \frac{\partial^2 \psi}{\partial x^2} + \frac{2m E}{\hbar^2} \psi = 0 \]

\[ E_n = \frac{n^2 \hbar^2}{8mL^2} \]

For 3-dimension,

\[ E_{n_x, n_y, n_z} = \frac{\hbar^2}{2m} \left( \frac{n_x^2 + n_y^2 + n_z^2}{L_x^2} + \frac{n_x^2 + n_y^2 + n_z^2}{L_y^2} + \frac{n_x^2 + n_y^2 + n_z^2}{L_z^2} \right) \]

\[ \Omega = \frac{\hbar^2}{2m} \left( n_x^2 + n_y^2 + n_z^2 \right) \]

\[ n_x^2 + n_y^2 + n_z^2 = \frac{4L^2 \hbar^2}{\Omega^2} \]

\[ \left( \frac{\hbar}{L^2} \right)^2 \rho^2 = \frac{\rho^2}{\Omega^2} \]

\[ \rho^2 = \left( \frac{\hbar}{L^2} \right)^2 \rho^2 \rightarrow 0 \]

where \( \rho \) = any vector from origin to any lattice point.

Allowed no. of integers in the range \( R \rightarrow R + dR \)

\[ dN = \frac{4 \pi R^2 \rho^2}{\Omega} \]

Since, \( R^2 = \left( \frac{\hbar}{2L} \right)^2 \rho^2 \)

\[ d\Omega dR = \left( \frac{2L}{\hbar^2} \right)^2 \rho^2 d\rho dp \]

\[ \Rightarrow \rho \rightarrow \left( \frac{2L}{\hbar} \right)^2 \rho \]
\[ \int \frac{1}{\sqrt{2}} \left( \frac{\alpha L}{L} \right)^2 \frac{1}{(2\hbar)} \, dp = \left( \frac{\alpha L}{L} \right) \, dp \]

Eqn 2 becomes,
\[ \frac{dn}{\delta} = \frac{1}{8} \frac{4\pi}{L} \left( \frac{L}{\hbar} \right)^2 \, p^2 \left( \frac{\alpha L}{L} \right) \, dp \]
\[ = \frac{4\pi L^3}{\hbar^3} \, p^2 \, dp \]

Since e\textsuperscript{-} have two spins hence allowed no. of wavefunctions in the momentum range.

\[ n = (p) \, dp = \frac{8\pi}{\hbar^3} \, p^2 \, dp \frac{V}{\frac{\hbar^3}{2}} \]

\[ \therefore p^2 = 2mE \]
\[ \delta p \, dp = \delta m \, dE \]
\[ dp = \frac{mdE}{p} \]

\[ \delta s \, dp = \frac{\frac{m^2}{\hbar^2}}{\sqrt{8mE}} \, dE \]

Eqn 3 may be written as,
\[ z \left( \frac{dE}{E} \right) = \frac{8\pi}{\hbar^3} \left( \frac{2m}{\hbar^3} \right) \frac{dE}{E} \]
\[ = \frac{4\pi}{\hbar^3} \left( \frac{2m}{\hbar^3} \right)^{3/2} \frac{E^{1/2}}{\hbar^3} \, dE \]
\[ = \frac{4\pi V}{\hbar^3} \left( \frac{2m}{\hbar} \right)^{3/2} \frac{E^{1/2}}{\hbar^3} \, dE \]
\[ E = \frac{\hbar^2}{8\pi^2 m} \left( \frac{8n}{8m} \right)^{2/3} \]

where \( \epsilon = \frac{4\pi N}{h^2} \left( 2m \right)^{3/2} \).

**Total no. of e-**

\[ N = \int_{0}^{E_f} z(E) \, dE \]

\( E_f = \) Fermi energy and it is defined as maximum k.e which e- can have at absolute zero of temp.

\[ \therefore N = \int_{0}^{E_f} C \, E^{1/2} \, dE \]

\[ = C \frac{E_f^{3/2}}{3} \]

\[ E_f = \left( \frac{8N}{8\pi^2 c} \right)^{2/3} \]

\[ = \frac{\hbar^2}{8\pi^2 m} \left( \frac{3N}{8\pi^2 V} \right)^{1/3} \]

\[ \therefore \frac{N}{V} = \rho_n \quad (\text{density of e-}) \]

\[ E_f = \frac{\hbar^2}{8\pi^2 m} \left( \frac{8N}{8\pi^2 V} \right)^{2/3} \]
Average Energy of free e⁻:

\[ \bar{E}_0 = \frac{1}{N} \int \bar{E} E_z \, dE \]

\[ \bar{E}_0 = \frac{1}{N} \int \frac{E E_z}{E_z} \, dE \]

\[ \bar{E}_0 = \frac{C}{N} \int \frac{E}{E_z} E_z^{5/2} \, dE \]

\[ \bar{E}_0 = \frac{8}{5} \frac{E_F}{E_z} \]

Effective mass of e⁻:

One e⁻ in the crystal interacts with the crystal lattice; therefore, its behaviour towards an external force is different from that of a free electron. This deviation of e⁻ behaviour is taken into account by considering the e⁻'s to have an effective mass \((m^*)\) rather than its free space mass \(m\).

The effective mass \(m^*\) depends on the nature of the crystal lattice and varies with the direction of motion of e⁻ in the lattice.
Let an e⁻ move when external field \( E \) is applied. Then the force acting on the e⁻ will be \( eE \).

Then work done by the force, \( W = eEdx \)

\[ W = eEv_gdt - (1) \]

(where \( v_g = \) group vel.)

\[ \Rightarrow v = \frac{eEv_g}{m} \]

Also, \( E = \frac{hv}{\lambda} = \frac{\hbar}{\lambda} \)

\[ dE = \frac{\hbar}{\lambda} dw = \frac{\hbar}{\lambda} dw \frac{dk}{dk} \]

\[ \Rightarrow \frac{h}{\lambda} v_g dk = (2) \]

from (1) and (2)

Equate eqn (1) and (2)

\[ eE v_g dt = \frac{h}{\lambda} v_g dk \]

\[ \Rightarrow dk = \frac{eEv}{\lambda} dt \]

From (2) \( v_g = \frac{\hbar}{\lambda} \frac{dE}{dk} \)

\[ \frac{d(v_g)}{dt} = \frac{\hbar}{\lambda} \frac{d^2E}{dk^2} \frac{dk}{dt} \]

\[ \Rightarrow \frac{d(v_g)}{dt} = \frac{\hbar}{\lambda} \frac{d^2E}{dk^2} \frac{dE}{dt} \]

\[ \therefore \frac{d(v_g)}{dt} = (\frac{\hbar}{\lambda})^2 \frac{d^2E}{dk^2} \frac{eE}{dt} \]
Again, \( v_0 = v \)

\[
\frac{dv}{dt} = \left( \frac{4\pi^2}{h^2} \frac{d^2E}{dk^2} \right) eE
\]

\[
\frac{dv}{dt} = \frac{1}{m^*} eE
\]

where, \( m^* = \left( \frac{4\pi^2}{h^2} \frac{d^2E}{dk^2} \right) \)

\[
\frac{dv}{dt} = \frac{1}{m^*} eE
\]

\[
F \downarrow \quad \text{force}
\]

\[
\text{mass}
\]

\[
\text{Conductivity} \quad \sigma -
\]

\[
\sigma = \eta_e e^2 \mu_e + \eta_h e^2 \mu_h
\]

where, \( \eta_e = e^- \text{ conc.} \)
\( \eta_h = \text{hole conc.} \)
\( \mu_e = e^- \text{ mobility} \)
\( \mu_h = \text{hole mobility} \)

\[
\text{Resistivity} \quad \rho
\]

\[
\rho = \frac{1}{\sigma}
\]

For intrinsic semiconductors
\[
\eta_e = \eta_h = \eta_i
\]
\[
\sigma = \eta_i e^2 (\mu_e + \mu_h)
\]
Concentration of free e⁻ & holes in semiconductors.

Let \( n \) be the no. of e⁻ per unit volume in the energy range \( E \) to \( E + dE \).

This is given by \( n(E) = g(E) f(E) \, dE \)

where \( g(E) = \text{no. of available quantum states of } e^- \)

\( f(E) = \text{Fermi function} \)

\[
\frac{1}{1 + e^{\left(\frac{E - E_F}{kT}\right)}}
\]

where \( E_F = \text{Fermi energy} \)

"Conduction band varies from \( E_g \) to \( \infty \)

\( \text{conc. of } e^- \text{ in conduction band is,} \)

\[
\eta_e = \int_{E_g}^{\infty} g(E) f(E) \, dE
\]

\[
= \int_{E_g}^{\infty} \frac{g(E)}{e^{\left(\frac{E - E_F}{kT}\right)} + 1} \, dE
\]

\( \therefore \) \( \frac{(E - E_F)}{kT} \gg 1 \)

\[
\eta_e = \int_{E_g}^{\infty} g(E) e^{-\left(\frac{E - E_F}{kT}\right)} \, dE
\]

\( \therefore \) \( \eta_e = k_e e^{-\left(\frac{E_g - E_F}{kT}\right)} \)

Similarly,

\( \eta_h = k_h e^{-\left(\frac{E_g - E_F}{kT}\right)} \)

for intrinsic semiconductors,

\( \eta_e = \eta_h \)
\[ E_g - E_F = E_g - E_F' \]
\[ E_g = E \]
\[ k_B e^\frac{(E_g - E_F)}{kT} = k_B e \]

Electron hole cone in intrinsic semiconductor.

Rate of combination

\[ R = \gamma n_e n_h \]

where \( \gamma = \text{const.} \) of proportionality

Under eqn,

rate of generation = rate of combination

\[ \therefore g = R = \gamma n_e n_h \]

In intrinsic,

\[ n_e = n_h = n \]

\[ \therefore g = R = \gamma n_e n_h = \gamma n^2 \]

\[ \therefore n^2 = n_e n_h \]
Polar and non-polar molecules

The molecules in which center of gravity of +ve and -ve charges coincide are known as non-polar molecule.

Simple moment of such molecules is zero. $\text{H}_2$, $\text{O}_2$, $\text{CO}_2$, $\text{CH}_4$, $\text{F}_2$.

These molecules have linear geometrical structure.

The molecules in which center of gravity of positive and negative charges do not coincide are known as polar molecules. Since center of gravity of +ve and -ve charges are separated by a distance of molecular dimension, they form an electric dipole. Therefore, net dipole moment of such molecules is non-zero. For e.g., $\text{H}_2\text{O}$, $\text{CH}_3\text{Cl}$, $\text{C}_6\text{H}_5\text{Cl}$.

Such molecules do not have symmetrical structure.

DIELECTRICS

Insulators are materials which have no free electron therefore they do not conduct electric current in presence of electric field. The insulators whose behavior gets modified in the presence of external electric field
are known as Dielectrics. Dielectrics are special types of insulators which are highly resistant to flow of electric current in them.

Dielectric Polarisation:

When a dielectric is placed in external electric field, its molecule acquire an electric dipole moment along the external field. This phenomenon in which dipole moment align along the direction of electric field is known as dielectric polarization.

Dielectric constant:

It is represented by $k$ or $\varepsilon_r$. It is also called relative permittivity.

$$\varepsilon_r = \frac{\varepsilon}{\varepsilon_0}$$

Where $\varepsilon_0 = $ permittivity of free space

$\varepsilon = $ "" material

Electric Polarisation vector:

It is also represented by $P$. It is also called dipole moment per unit volume. It is defined as vector field that express the density of permanent or induced dipole moment.
electric moment in electric material. Its unit is C/m². \( \vec{P} \) is proportional to strength \( \vec{E} \) of external electric field.
\[
\vec{P} \propto \vec{E}^2 = \vec{\kappa}_e \vec{E}^2
\]
where \( \vec{\kappa}_e \) = Electric susceptibility.

Electric displacement vector \((D)\)
\[
\vec{D} \propto \vec{E}^2 = \vec{\varepsilon} \vec{E}\]

\(\vec{D} \) or \( \vec{F} \) and \( \vec{\varepsilon} \) are surface charged density of bound and free charge, then
\[
\vec{P} = \vec{\varepsilon}_b
\]
\[
\vec{D} = \vec{\varepsilon}_f
\]

\(\vec{P} = \alpha \vec{E}\)
where \( \alpha \) = Electric polarizability of dielectric material.

Relation b/w \( \vec{D}, \vec{E} \) & \( \vec{P} \)
Consider electric polarization of dielectric slab. Insulated slab plates of capacitor. Let \( \vec{\varepsilon}_b \) and \( \vec{\varepsilon}_f \) are surface charged density of free and bound charge present on capacitor plate and dielectric slab respectively.
Let \( E_f \) & \( E_b \) be the respective electric field strength of free charges and bound charges. Then the magnitude of \( E_f \) and \( E_b \) are given by:

\[
E_f = \frac{\sigma_f}{\varepsilon_0}
\]

\[
E_b = \frac{\sigma_b}{\varepsilon_0}
\]

Since they are oppositely directed, hence the net electric field is given by:

\[
E = E_f - E_b = \frac{\sigma_f}{\varepsilon_0} - \frac{\sigma_b}{\varepsilon_0}
\]

or,

\[
\sigma_f - \sigma_b = \varepsilon_0 E
\]

or,

\[
D - P = \varepsilon_0 E
\]

In vector form,

\[
\vec{D} - \vec{P} = \varepsilon_0 \vec{E}
\]

or,

\[
\vec{D} = \vec{P} + \varepsilon_0 \vec{E}
\]

In above, relation 2)

1) \( D \) is related to free charges and it can be represented by lines of electric displacement.
2) The lines of \( P \) begin and end on bound charges.
3) \( E \) is related to both free charges...
and bound charges.

Relationship between $\chi_e$ and $K$.

Dielectric susceptibility and dielectric constant.

1. $\overrightarrow{D} = \varepsilon_0 \overrightarrow{E} + \overrightarrow{P}$
2. Also $\overrightarrow{D} = \varepsilon \varepsilon_0 \overrightarrow{E}$
3. $\overrightarrow{P} = \chi_e \varepsilon_0 \overrightarrow{E}$

Putting 2 and 3 in 1

$\varepsilon \varepsilon_0 \varepsilon \overrightarrow{E} = \varepsilon_0 \overrightarrow{E} + \chi_e \varepsilon_0 \overrightarrow{E}$

Also, $K = \frac{\varepsilon}{\varepsilon_0}$

$\Rightarrow \varepsilon = \varepsilon_0 K$

Putting 3 in 4

$\varepsilon_0 K \varepsilon \overrightarrow{E} = \varepsilon_0 \overrightarrow{E} + \chi_e \varepsilon_0 \overrightarrow{E}$

Therefore, $K = 1 + \frac{\chi_e}{\varepsilon_0}$

Therefore, $\chi_e = (K-1) \varepsilon_0$

Or, $\overrightarrow{P} = \chi_e \varepsilon_0 \overrightarrow{E}$

Or, $\overrightarrow{P} = (K-1) \varepsilon_0 \overrightarrow{E}$
Gauss Law in Dielectric

This law states that the surface integral of the electric displacement vector over a closed surface that encloses charges is equal to the free charge. Mathematically,

\[ \oint \vec{D} \cdot d\vec{s} = \Phi_f \]

where \( \vec{D} \) = electric displacement vector, \( \Phi_f \) = free charge.

Let \( q_p \) and \( q_b \) are free and bound charges on the capacitor plate and dielectric slab respectively. Then according to Gauss law

\[ \oint \vec{E} \cdot d\vec{s} = \frac{1}{\varepsilon_0} (q_p - q_b) \]

Let \( E \) be the electric field. Let \( E_0 \) be the electric strength on the capacitor plate, in the absence and presence of the dielectric slab.

Then dielectric constant \( K = \frac{E_0}{\varepsilon_0} \)

Also, \( E_0 = \frac{q_p}{A \varepsilon_0} \)

\[ K = \frac{q_p}{A \varepsilon_0 E} \]

\[ E = \frac{q_p}{A \varepsilon_0 K} \]
\[ E_f - E_b = \frac{q_f}{A \varepsilon_0} \]

\[ \frac{E_f}{\varepsilon_0} - \frac{E_b}{\varepsilon_0} = \frac{q_f}{A \varepsilon_0} \]

\[ \frac{q_f}{A \varepsilon_0} - \frac{q_b}{A \varepsilon_0} = \frac{q_f}{A \varepsilon_0} \]

\[ \frac{q_f}{A \varepsilon_0} - \frac{q_b}{A \varepsilon_0} = \frac{q_f}{A \varepsilon_0} \]

\[ \frac{q_f}{A \varepsilon_0} - \frac{q_b}{A \varepsilon_0} = \frac{q_f}{A \varepsilon_0} \]

\[ q_f - q_b = \frac{q_f}{k} \]

\[ q_f - q_b = \frac{q_f}{k} \]

Putting in eq (1)

\[ \text{eq (1) becomes} \]

\[ \oint \mathbf{E} \cdot d\mathbf{l} = \frac{q_f}{k} \]

\[ \oint \mathbf{E}_0 \cdot d\mathbf{l} = q_f \]

\[ \oint \mathbf{D} \cdot d\mathbf{s} = q_f \]

Type of magnetic materials

1) Diamagnetic materials → These materials are...
Slightly depleted by magnetic field and material does not exhibit magnetic properties when external field is removed. In this all e\(^{-}\)s are paired and therefore they have no permanent net magnetic moment per atom. They have very weak susceptibility. For e.g. copper, silver, gold.

2) Paramagnetic materials - In this case at least one of the material have not magnetic moment due to unpaired e\(^{-}\)s in partially filled orbitals. Paramagnetic properties are due to the presence of these unpaired e\(^{-}\)s and form realignment of e\(^{-}\)s caused by external magnetic field. These materials are slightly attracted by M.F. and materials don't lose these magnetic properties when M.F. field is removed. They have positive susceptibility. For e.g. magnesium, molybdenum, lithium.

3) Ferromagnetic materials - They have large and positive susceptibility due to pair of unpaired e\(^{-}\)s. They exhibit strong attraction to a magnetic field and are able to retain their magnetic properties even after external field is removed. These materials have very few unpaired e\(^{-}\)s. For e.g. iron, nickel, cobalt.
1) Ferromagnetic materials:
   In these materials, magnetic structure is composed of two magnetic sub-lattices whose spin moments are oriented in opp. direction, for e.g., Fe, Co, Ni, FeS.

2) Antiferromagnetic materials:
   In this, two sub-lattices have exactly equal and opp. spin orientation, therefore the net magnetic moment of these materials is zero. For e.g., FeS.
Clausius - Mosotti Equation

For non-polar dielectrics, the molecular electric field is given by:

\[ E_m = \frac{E + \rho}{3\varepsilon_0} \]

This eqn gives the relationship between molecular polarisability \( \alpha \) and dielectric constant \( K \). It is valid for non-polar molecules.

\[ E_m = E + \rho \]

where \( \rho = \) polarisation \( \frac{3}{3\varepsilon_0} \)

\( \rho \) is induced dipole moment.

\[ \rho = K \varepsilon_0 E \]

It is no. of molecules per unit vol.

Their polarization \( \rho \) is:

\[ \rho = N \rho_m \]

\[ \rho_m = N \alpha \left( \frac{E + \rho}{3\varepsilon_0} \right) \]

\[ \rho = (K-1) \varepsilon_0 E = N\alpha \left( E + \frac{(K-1)\varepsilon_0 E}{3\varepsilon_0} \right) \]

\[ \rho_m = (K-1) \varepsilon_0 = N\alpha \left[ 1 + \frac{(K-1)}{3} \right] \]

\[ \rho_m = \frac{(K-1)}{\varepsilon_0} = \frac{N\alpha}{\varepsilon_0} \left[ \frac{3 + K - 1}{3} \right] \]

\[ (K-1) = \frac{N\alpha}{\varepsilon_0} \left[ \frac{3 + K - 1}{3} \right] \]
\( \sigma_I = \frac{N \sigma}{3 \varepsilon_0} \left( \frac{1}{k+2} \right) \)

\( \varepsilon \), where \( \varepsilon = \frac{3 \varepsilon_0}{N} \left( \frac{k-1}{k+2} \right) \) is the Clausius–Mosotti Equation.