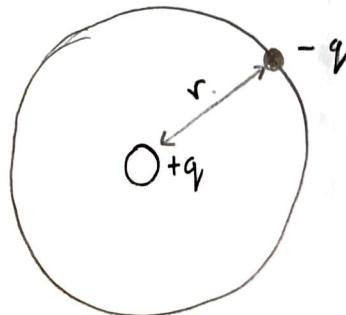


Bohr's Model - Ch 2.

- Electron's exist in a stable, circular orbit.
- ∴ Implies that orbiting electrons do NOT give off radiation.
(classical electromagnetism).
- $\Delta E = E_2 - E_1$, can shift to higher or lower energies.
- Angular momentum $P_0 = nh$, $n = 1, 2, 3 \dots$

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

(Electron orbiting around a proton).



→ We can equate the electrostatic forces between the charges to the centripetal force

$$\therefore F_e = \frac{kq_1 q_2}{r^2} \text{ since same charge } F_e = \frac{kq^2}{r^2}$$

$$\text{or } k = \frac{1}{4\pi\epsilon_0} \quad \therefore \boxed{F_e = \frac{-q^2}{kr^2}} \text{ since electron charge negative.}$$

$$\therefore \boxed{F_c = \frac{mv^2}{r}}$$

$$\therefore F_c = F_e$$

$$\frac{mv^2}{r} = \frac{kq^2}{r^2} \Rightarrow mv^2 = \frac{kq^2}{r} \quad \left. \begin{array}{l} E_T = KE + PE \\ E_T = \frac{1}{2}mv^2 + \frac{kq^2}{r} \end{array} \right\} \quad \therefore E = \frac{1}{2} \left(\frac{kq^2}{r} \right) + \frac{kq^2}{r}$$

$$(1) \quad \quad \quad E = \frac{kq^2}{r} \left(-\frac{1}{2} \right) = \boxed{-\frac{1}{2} \frac{kq^2}{r}} \quad (2)$$

Angular momentum ∴ (need to quantised)

$$L = mrv$$

$$\therefore mrv = nh \Rightarrow r = \frac{nh}{mr} \quad \left. \begin{array}{l} \text{Sub into (1)} \therefore mv^2 = \frac{kq^2}{r} \\ \text{and } \left(\frac{n^2 h^2}{m^2 r^2} \right) = \frac{kq^2}{r^2} \Rightarrow \frac{n^2 h^2}{mr} = kq^2 \end{array} \right\}$$

$$\boxed{r = \frac{n^2 h^2}{mkq^2}} \quad \text{Bohr radius} \quad (3)$$

$$\therefore \text{Sub (3) into (1).}$$

$$E_n = -\frac{1}{2} \frac{k^2 q^4 m_e}{h^2} \left(\frac{1}{n^2} \right)$$

$$\text{Energy levels for hydrogen} \quad (4)$$

$$E_n = -\frac{1}{2} \frac{\frac{k^2 q^4}{n^2 h^2}}{m_e} \quad \text{sub (4) into } E_2 \text{ & } E_1$$

$$\therefore \frac{1}{n} = \frac{E_2 - E_1}{2\pi\hbar c}$$

$$\left(h = \frac{\hbar}{2\pi} \right) \quad \therefore \frac{1}{n} = \frac{\left(-\frac{1}{2} \frac{m_e k^2 q^4}{h^2} \cdot \frac{1}{n_2^2} \right) - \left(-\frac{1}{2} \frac{m_e k^2 q^4}{h^2} \cdot \frac{1}{n_1^2} \right)}{2\pi\hbar c} \quad \left. \begin{array}{l} \frac{1}{n} = \left(\frac{1}{n_2^2} - \frac{1}{n_1^2} \right) \left(\frac{m_e k^2 q^4}{4\pi\hbar^3 c} \right) \\ L_D \end{array} \right)$$

$$\therefore \frac{1}{n} = \left(\frac{1}{n_2^2} - \frac{1}{n_1^2} \right) \left(\frac{1}{2} \frac{m_e k^2 q^4}{h^2} \right) \left(\frac{1}{2\pi\hbar c} \right)$$

$$\therefore \frac{1}{n} = R_H \left(\frac{1}{n_2^2} - \frac{1}{n_1^2} \right) \quad \text{Rydberg constant}$$

Heisenberg Uncertainty principle

↳ Uncertainty in position & momentum of a particle

$$(\Delta x)(\Delta p) \geq \frac{\hbar}{2}$$

↳ Uncertainty in energy & time

$$(\Delta E)(\Delta t) \geq \frac{\hbar}{2}$$

→ Given probability density function $P(x)$ for 1-D [continuous]

$$\int_{-\infty}^{\infty} P(x) dx = 1. \quad \begin{matrix} \rightarrow \text{Normalised} \\ [\int = \text{unity}] \end{matrix} \quad (1)$$

→ Average value of a function $f(x)$

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x) P(x) dx. \quad (2)$$

→ If not Normalised.

$$\langle f(x) \rangle = \frac{\int_{-\infty}^{\infty} f(x) P(x) dx}{\int_{-\infty}^{\infty} P(x) dx}.$$

Schrödinger Wave Equation

Basic Postulates

1) Each particle in a physical system is described by a wave function $\psi(x, y, z, t)$.

This function & its space derivatives ($\frac{\partial \psi}{\partial x} + \frac{\partial \psi}{\partial y} + \frac{\partial \psi}{\partial z}$)
are continuous, finite, and single valued

2) For every classical observable, there corresponds a linear, Hermitian, quantum mechanical operator.

Classical variable	Quantum operator
x	x
$f(x)$	$f(x)$
$p(x)$	$\frac{ih}{j} \frac{\partial}{\partial x}$
E	$-\frac{h^2}{j} \frac{\partial^2}{\partial t^2}$

& similarly for the other directions

3) The probability of finding a particle with wavefunction ψ in the volume $dx dy dz$ is $|\psi^* \psi| dx dy dz$

Product: $\psi^* \psi$ is normalised.

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

$$\int_{-\infty}^{\infty} [f(x)]^2 dx = C \quad \begin{matrix} \text{real} \\ \text{number} \end{matrix}$$

& Average value $\langle Q \rangle$ of any variable Q :

$$\langle Q \rangle = \int_{-\infty}^{\infty} \psi^* Q_{op} \psi dx dy dz$$

$$C < \infty$$

like e^{-x^2}

∴ Classical equation of the energy of a particle

$$KE + PE = \text{Total Energy}$$

$$\therefore \frac{p^2}{2m} + V = E$$

According to postulate (2); they are allowed to operate on the wave function ψ .

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} + V(x) \psi(x, t) = \frac{\hbar}{j} \frac{\partial \psi(x, t)}{\partial t} \quad (1)$$

} Both include
space &
time dependence,

IN 3-D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi = -\frac{\hbar}{j} \frac{\partial \psi}{\partial t} \quad (2)$$

where: $\nabla^2 \psi$ is $\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}$

• Let $\psi(x, t) = \psi(x) \phi(t)$ → substitute into (1).

$$\therefore -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} \phi(t) + V(x) \psi(x) \phi(t) = -\frac{\hbar}{j} \psi(t) \frac{d \phi(t)}{dt}$$

Separate variables to obtain time-dependent equation (1-D)

$$\frac{d \phi(t)}{dt} + \frac{jE}{\hbar} \phi(t) = 0$$

2 Time-independent

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

* Note: The operational operator of $(\partial/\partial x)^2$ is $\delta^2/\delta x^2$; $j(j)^2 = -1$

Given that $\psi = A \exp(jk_x x)$ what is the expectation value of p_x , x -component of momentum

$$\Rightarrow \psi = A \exp(jk_x x)$$

From the postulate (3)

$$\langle p_x \rangle = \int_{-\infty}^{\infty} \psi^* Q_{op} \psi \quad \therefore (\exists) \langle p_x \rangle = \int_{-\infty}^{\infty} A \exp(-jk_x x) \left(\frac{\hbar}{j} \frac{d}{dx} \right) A \exp(jk_x x) dx$$

Quantum operator
of momentum

Since NOT normalised ..

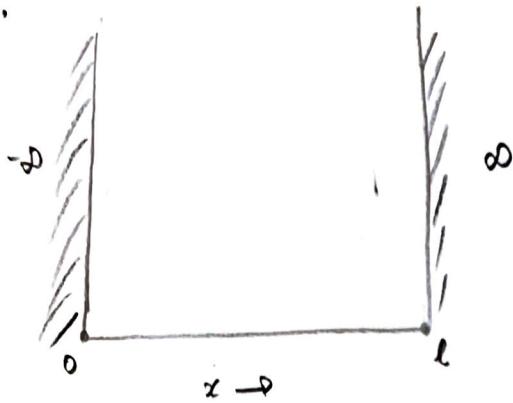
$$\begin{aligned} \langle p_x \rangle &= \frac{\int_{-\infty}^{\infty} A e^{-jk_x x} \left(\frac{\hbar}{j} \frac{d}{dx} \right) A e^{jk_x x} dx}{\int_{-\infty}^{\infty} \psi^* \psi} \quad \left[\frac{\psi^* Q_{op} \psi}{[\psi^* \psi]} \right] \\ &= \frac{\int_{-\infty}^{\infty} A e^{-jk_x x} \left(\frac{\hbar}{j} \frac{d}{dx} \right) A e^{jk_x x} dx}{\int_{-\infty}^{\infty} |A|^2 e^{-jk_x x} \cdot e^{jk_x x}} = \int_{-\infty}^{\infty} \frac{\hbar}{j} \frac{d}{dx} = (\hbar k_x), // \end{aligned}$$

Note: If we try to integrate them, both numerator & denominator tend to infinity.,

Because an ideal plane wave is not normalizable. wave function.

Trick: Use $1/2 \leftrightarrow (-1/2)$, L cancels out, & then $L \rightarrow \infty$.

Particle In A Box Problem



$$V(x) = \begin{cases} 0 & \text{if } 0 < x < l \\ \infty & \text{otherwise.} \end{cases}$$

∴ Schrödinger's Equation:

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

$$\therefore \frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) \quad \left. \begin{array}{l} \text{solving diff. equation} \\ \hline \end{array} \right.$$

$$\therefore \text{Solution} \Rightarrow \psi(x) = A\cos(kx) + B\sin(kx)$$

$$\boxed{k = \frac{\sqrt{2mE}}{\hbar}}$$

Using Boundary conditions:

$$\psi(x \leq 0) = 0 \rightarrow \psi(0) = 0$$

$$\psi(x > l) = 0 \rightarrow \psi(l) = 0$$

$$\therefore \psi(0) = A\cos(k \cdot 0) + B\sin(k \cdot 0) = A \rightarrow A = 0.$$

$$\therefore \psi(l) = B\sin(kl) = 0 \quad \therefore kl = \sin^{-1}(0) = n\pi \quad \begin{array}{c} \text{Diagram of a wave function} \\ \text{with nodes at } x=0 \text{ and } x=l \\ \text{and } n \text{ peaks.} \end{array}$$

$$\therefore \boxed{k = \frac{n\pi}{l}}$$

quantum number

$$\therefore \psi(x) = B\sin\left(\frac{n\pi x}{l}\right) \quad n = 1, 2, 3, 4, \dots$$

$$\frac{n\pi}{l} = \frac{\sqrt{2mE}}{\hbar} \Rightarrow \frac{n^2\hbar^2\pi^2}{l^2} = 2mE \quad \therefore \boxed{E_n = \frac{\hbar^2 n^2}{8ml^2}}$$

To get B? (Use postulate 3)

$|\Psi_n(x)|^2 dx = \Psi^*(x) \Psi(x) dx$ = Probability that particle position $\leq x + dx$

$$\therefore \int_{-\infty}^{\infty} \Psi^*(x) \Psi(x) dx = 1$$

$\therefore \Psi(x) = 0$ if $x \leq 0$ or $x \geq l$

$$(=) 1 = \int_0^l [B \sin(n\pi/l)]^* [B \sin(n\pi/l)] dx$$

$$1 = B^2 \int_0^l \sin^2(n\pi/l) dx$$

$$\sin^2(kx) = \frac{1}{2}(1 - \cos(2kx)) \quad \text{[Identity]}$$

$$\therefore 1 = \frac{B^2}{2} \int_0^l 1 - \cos(2n\pi/l) dx$$

$$\frac{2}{B^2} = \left[\left(x - \frac{l}{2\pi n} \sin\left(\frac{2n\pi}{l}\right) \right) \right]_0^l$$

$$\frac{2}{B^2} = \left[l - \frac{l}{2\pi n} \cancel{\sin(2\pi n)} \right] - \left[0 - \frac{l}{2\pi n} \cancel{\sin(0)} \right]$$

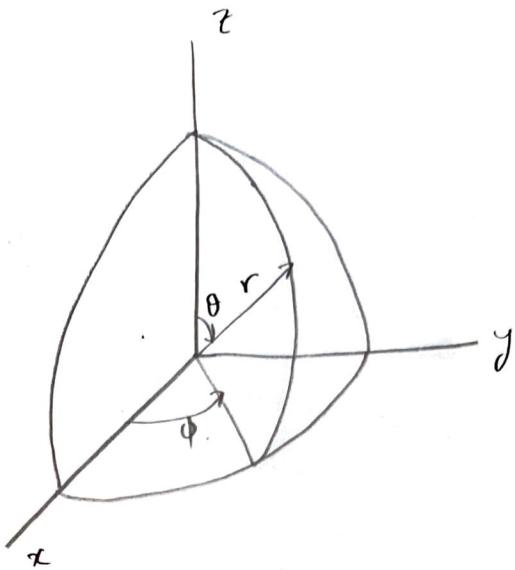
$$\therefore \frac{2}{B^2} = l \quad (\Rightarrow B = \sqrt{\frac{2}{l}})$$

④ B = normalization constant \circledast

$$\boxed{\Psi_n(x) = \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi x}{l}\right)}$$

Hydrogen Atom Solution

- Since problem is spherically symmetric, the spherical coordinate system is used.



Schrödinger equation in 3-D

$$\frac{-\hbar^2}{2m} \nabla^2 \psi + V\psi = -\frac{\hbar}{i} \frac{\partial \psi}{\partial t}$$

→ Replaced with $V(r, \theta, \phi) = V(r) = \frac{kq^2}{r}$

- After separation of variable ($\Rightarrow \psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$)
∴ Expect 3 quantum numbers associated with each of 3 parts

$\therefore \phi$ -dependent equation after separation of variables is:

$$\frac{d^2\phi}{d\phi^2} + m^2\phi = 0 \quad \therefore m \text{ is a quantum number}$$

$$\Phi_m(\phi) = Ae^{jm\phi}$$

$$\therefore A = ?$$

$$\int_0^{2\pi} \Phi_m^*(\phi) \Phi_m(\phi) d\phi = 1$$

$$\therefore \int_0^{2\pi} Ae^{-jm\phi} \cdot e^{jm\phi} = A^2 \int_0^{2\pi} d\phi = 2\pi A^2 //$$

$$(=) A = \frac{1}{\sqrt{2\pi}} \quad 2 (=) \Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{jm\phi}$$

since ϕ is repeated every 2π ϕ should repeat also.
This occurs when m is an integer including negatives & 0
 $m = -3, -2, \dots, 1, 2, 3, \dots$

Similarly for $\underbrace{R(r), \Theta(\theta)}_{\downarrow}$ \rightarrow quantum number $= l = 0, 1, 2, \dots, n-1$
quantum number $= n > 0$

Conclusion:

$$\Psi_{nlm}(r, \theta, \phi) = R_n(r) \Theta_l(\theta) \Phi_m(\phi) //$$

Restrictions: [principal quantum number].

$$n = 1, 2, 3, \dots, (n-1)$$

$$l = 0, 1, 2, 3, \dots, l$$

$$m = -l, \dots, -2, -1, 0, +1, +2, \dots, +l$$

$$\oplus \quad \pm \frac{n}{2} \text{ (spin)}$$

Ch 3 - Energy Bands & Charge Carriers in Semiconductors

- Difference between an electron in an atom & an electron in a solid is that:

→ Electrons in a solid, have a range, or band of available energies
 This is because in solid, the wave functions of electrons overlap
 \therefore alter the Schrödinger equation boundary conditions & potential energy.

Bonding Forces in Solids

- Ionic Bonding
- Metallic Bonding
- Covalent Bonding

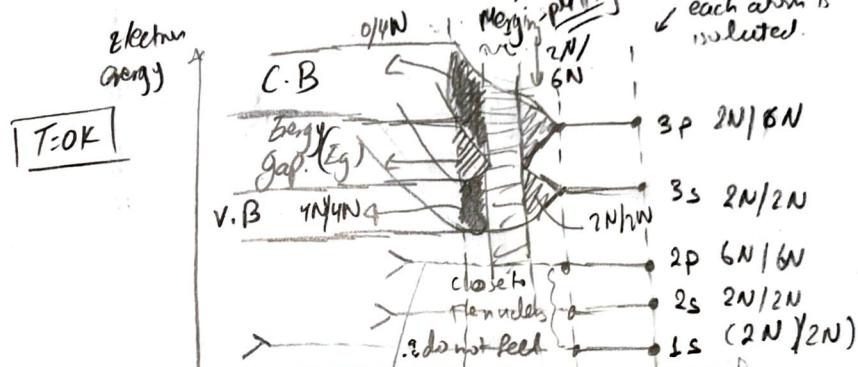
Energy Bands

As the spacing between atoms decreases, electron wave functions overlap.
 Due to Pauli's exclusion principle, this must be at most 1 electron per level. after there is a splitting of discrete energy levels of isolated atoms, into new levels belonging to the pair rather than individual atoms.

For example Silicon

Si - 14

$1s^2$	→ Inner $2/2$
$2s^2 \quad 2p^6$	→ Middle $8/8$
$3s^2 \quad 3p^2$	Outer $4/8$ valence.



Note③:

In metals, energy band overlap is partially filled.

∴ energy states are determined.

∴ electrons are freely to move under influence of an electric field.

Pauli exclusion principle
 \therefore splitting.

($T=0K$)
 (Interatomic
 distance)
 Si atoms | N: silicon atoms

Note④: At $0K$ → valence band is completely filled

Note⑤: At $0K$ → valence band is completely filled

• Band gap (E_g) = 1.1 eV for Silicon.

The number of electrons available for conduction can greatly be increased by thermal or optical energy.

Note⑥: In semiconductors

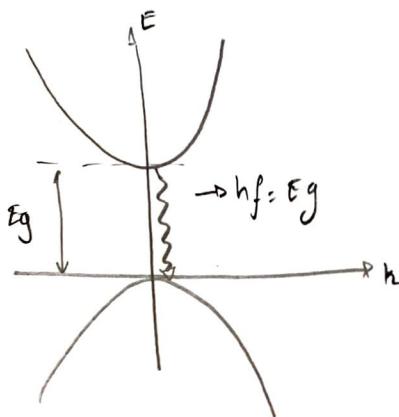
Direct & Indirect Semiconductors

→ The wave function of the electron is assumed to be in the form of a plane wave moving, eg, in the x -direction with propagation constant \vec{k} (wave vector)
 \therefore Space-dependent

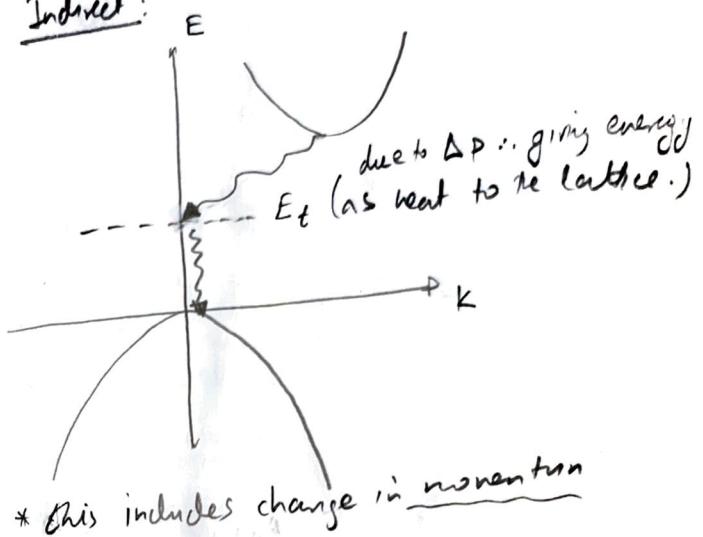
$$\psi_{\vec{k}}(x) = U(k_x, x) e^{i k_x x}$$

→ where $U(k_x, x)$ modulates the wave function according to the periodicity of the lattice.

Direct:



Indirect:



Example:
 Assume U is constant, show that x -component of the electron momentum in the crystal is given by $\langle p_x \rangle = \hbar k_x$

$$\begin{aligned} \int_{-\infty}^{\infty} \psi^* \psi \frac{1}{2m} \nabla^2 \psi = \int_{-\infty}^{\infty} U^2 e^{-jk_x x} \frac{i}{j} \frac{\partial}{\partial x} (e^{ik_x x}) dx \\ \int_{-\infty}^{\infty} \psi^* \psi = \int_{-\infty}^{\infty} U^2 dx \end{aligned}$$

$$= \frac{\hbar k_x \int_{-\infty}^{\infty} U^2 dx}{\int_{-\infty}^{\infty} U^2 dx} = \hbar k_x$$

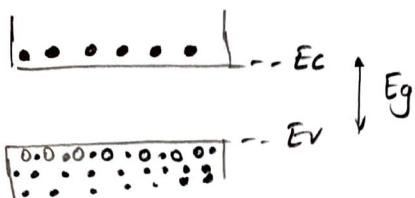
* Note: This results that (E, k) diagrams can be considered plots of electron energy vs momentum with scaling factor of \hbar

Charge Carriers in Semiconductors

Electrons & Holes

- As $T \downarrow$ of a semiconductor from OK some electrons in the valence band receive enough thermal energy to be excited across the band gap to the conduction band.

(eg)



• electrons } Electron-hole pair (EHP)
• holes

For example: In silicon (Si), at room temperature 10^{10} EHP/cm³ compared to the Si atom density of 5×10^{22} atoms/cm³

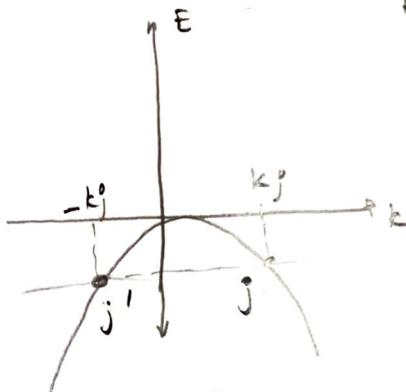
∴ some electrons are free to move about in many available empty states

* Charge transport in the valence band can be simulated by keeping track of the holes

In a filled band

- For every electron with a given velocity there is an equal & opposite electron moving elsewhere in the band
- If we apply an electric field, the net current is zero
[electron(j) with velocity (v_j) \leftrightarrow electron (j') with velocity ($-v_j$)]

$k \& p$ (momentum)



[valence band?
filled]

∴ In a filled band:

$$I = n A q v, \quad n = \text{charge carrier density (N/cm}^3\text{)}$$

$q = \text{charge} \therefore -q \text{ for electron}$

$$\frac{I}{A} = n q v$$

$$J = (-q) \sum_i^n v_i = 0.$$

• If we create a hole by removing the j^{th} electron.

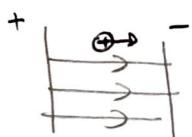
Now

$$J = (-q) \sum_i v_i - (-q) v_j \text{ (electron missing)}.$$

$J = +q v_j$ (\Rightarrow) In other words, the current contribution of holes is equivalent to that of a positively charged with velocity (v_j) \rightarrow that of a missing electron.

\Rightarrow Charge transport is actually due to the motion of the new uncompensated electron (j')

Electric field notes



holes move in the direction of the electric field.
electrons move opposite the direction of E field.

*Note: Hole energy ↑ oppositely to the electron energy.

because the carriers have opposite charge.

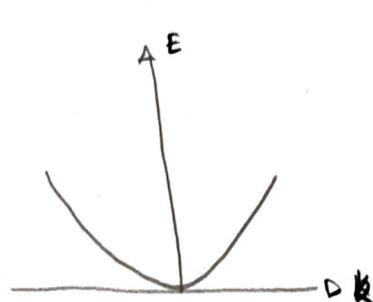
\therefore Lowest energy state available \rightarrow top of valence band.

\Rightarrow In contrast, conduction band electrons are found at the bottom of the conduction band.

\rightarrow electrons move to most stable state \therefore ground state.

Effective Mass

- Electrons in a crystal are not completely free, but instead interact with the periodic potential lattice.
- As a result, their "wave-particle" motion cannot be expected to be the same as an electron in free space.
- ∴ Alter particle mass to take into account most of the influences.
- ⇒ (E, k) relation of a free electron related to the electron mass.



$$p = mv = \hbar k$$

$$\therefore E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

$$\therefore E \propto \frac{1}{m}$$

$$\left(\Rightarrow \frac{d^2 E}{dk^2} = \frac{\hbar^2}{m} \right)$$

$$\left(\Rightarrow m^* = \frac{\hbar^2}{d^2 E / dk^2} \right) \quad m^* = \text{effective mass}$$

→ Why effective mass is different from true mass

◦ (N2L) $\rightarrow \Delta p$:

$$F = m \cdot a = \frac{dp}{dt} = \frac{d(mv)}{dt} = \text{Force.}$$

↳ An electron in the crystal experiences a total force $F_{\text{INT}} + F_{\text{ext}}$

F_{INT} = internal periodic crystal forces

F_{ext} = External force applied.

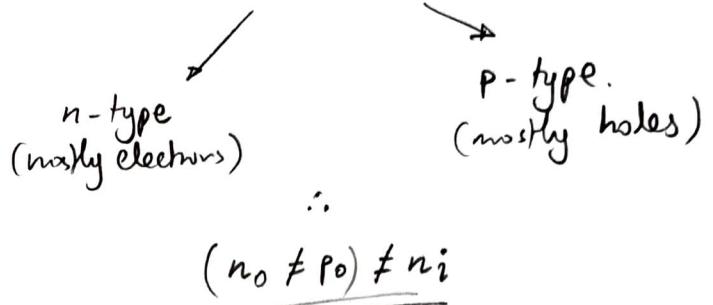
$F_{\text{ext}} - d(m_N^* v) / dt =$, Periodic crystal potential varies for different semiconductors

Intrinsic Material

- Semiconductors crystal with no impurities or lattice defects
 - ↳ At 0 K no charge carriers - valence band filled with electrons
- conduction band empty
 - As $T \uparrow$, EHP are created \rightarrow only charge carriers in the material.
 - Since electrons & holes are created in pairs
 - conduction band electron concentration (n) [$1/\text{cm}^3$] = hole concentration (p) [$1/\text{cm}^3$]
 - $\therefore \boxed{n = p = n_i} \rightarrow$ for intrinsic material
 - \rightarrow At a given temperature, there is a certain concentration of electron-hole pairs (n_i)
 - \therefore At steady state carrier concentration maintained
 - Recombination occurs \rightarrow When electron in the conduction band makes a transition (direct or indirect) to an empty state (hole) in the valence band \therefore Annihilation occurs [photon created]
 - (=) g_i (generation rate of EHP/ cm^3) = recombination rate (r_i)
 - $\therefore \boxed{g_i = r_i}$
 - Since rates are temperature dependent
 - $\therefore r_i = \alpha_r n_0 p_0 = \alpha_r n_i^2 = g_i$
 - where α_r is a constant of proportionality which depends on the particular mechanism by ~~which~~ which recombination occurs.
- As $T \uparrow$, $g_i \uparrow \therefore$ new carrier concentration (n_i) established.
such that the higher r_i is balanced with the generation

Extrinsic Material

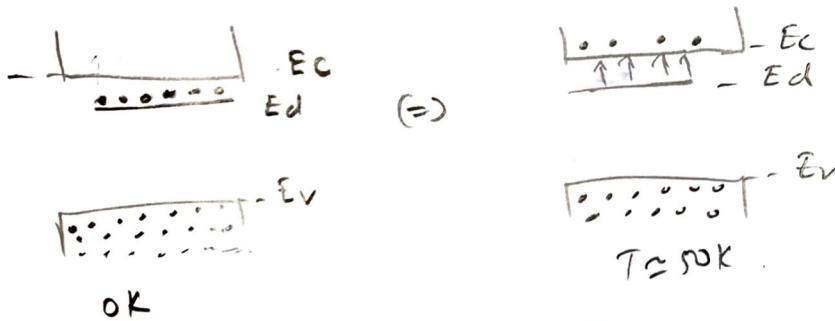
- In addition to the intrinsic carriers generated normally.
- ↳ can create carriers in semiconductors by introducing impurities
[Process called: doping] \therefore Crystal can be altered
(=) predominance of either electrons or holes.



→ When impurities or lattice defects are introduced into a perfect crystal additional levels are created in the energy band structure.
(usually within band gap).

→ For n-type:

- Impurities from column V of periodic table (P, As, Sb) ..
- ↳ introduce energy level very near the conduction band of Ge or Si.
↳ filled with electrons at 0K \therefore little energy required.

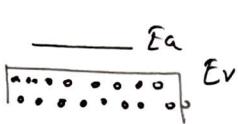


- $E_d = \text{impurity level} \rightarrow \text{Donor level}$
- ↳ Column V impurities are called donor impurities

\therefore In general: $n_o \gg (n_i, p_0)$ At room temperature.

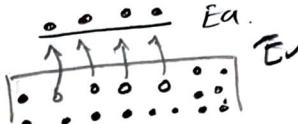
• For p-type:

→ Impurities from column III (B , Al , Ga , In)
↳ introduce energy level near the valence band.



$$T = 0K$$

(=)



$$T \approx 50K$$

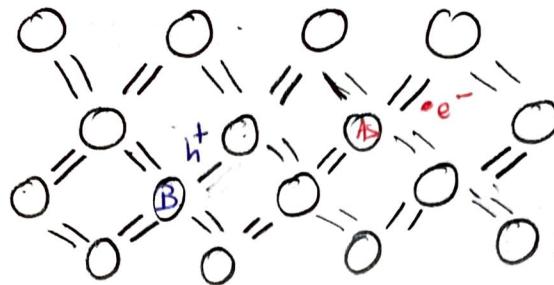
E_a = impurity level \rightarrow Acceptor level

✗ Column III are called acceptor impurities

$$\therefore p_0 \gg (n_i, n_o)$$

[hole concentration (p_0) is much greater than the conduction band electron concentration (n_o)]

• In a Silicon (Si) crystal. (pg 79). ④ As has 5 electrons, only 4 are needed for covalent bonding



} donor & acceptor atoms in the covalent bonding model of Si crystal.

→ Energy required to excite the ^④ fifth electron of a donor atom into the conduction band → Donor binding energy

∴ Total energy of the electron in the n_{th} orbit. (Bohr model).

$$E_n = KE + PE = \frac{m\omega^2 r^4}{2\epsilon^2 h^2}$$

$$\boxed{n=1}$$

* Note: Hydrogen atom approximation

∴ It must be modified from the free space of Hydrogen ($4\pi\epsilon_0$) to:

$$1K = 4\pi\epsilon_0\epsilon_r \quad \epsilon_r = \text{relative dielectric constant of semiconductor material.}$$

$$\therefore E_D = \frac{m^* g^4}{2 [4\pi\epsilon_0\epsilon_r]^2 h^2} \quad //$$

* Note: We refer to the small number of holes in the n-type material as minority carriers & the relatively large number of conduction band electrons as major carriers.

Q) If Si is doped with As
At 0K = $n_i = 10^{10} / \text{cm}^3$ doped with 10^{15} As/cm^3

electron concentration changes by 5 order of magnitude.

∴ Resistivity of Si at $2 \times 10^5 \Omega \text{-cm}$ changes to $5 \Omega \text{-cm}$ with doping.

④ ONLY 1 type of carrier dominates //

Carrier Concentrations

The Fermi-level :

→ Electrons in solids obey Fermi-Dirac statistics

↳ Distribution of electrons over a range of allowed energy levels at thermal equilibrium: is:

$$f(E) = \frac{1}{1 + e^{(E - E_F)/kT}}$$

} probability an available energy state will be occupied by an electron.

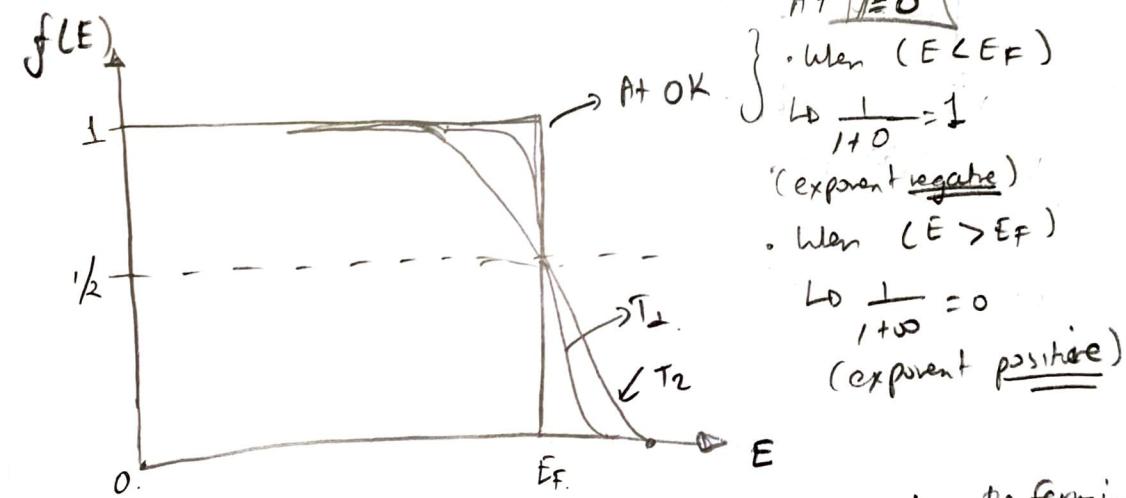
• k = Boltzmann's constant ($8.62 \times 10^{-5} \text{ eV/K} = 1.38 \times 10^{-23} \text{ J/K}$)

• E_F = Fermi level.

$$\Leftrightarrow \text{At } E = E_F \Rightarrow f(E_F) = \frac{1}{1 + e^{(E_F - E_F)/kT}} = \frac{1}{1+1} = \frac{1}{2}$$

∴ An energy state at the Fermi level has a probability of $\frac{1}{2}$ of being occupied by an electron

Fermi-Dirac Distribution Function



At $T \neq 0$

• When $(E < E_F)$
↳ $\frac{1}{1+0} = 1$
(exponent negative)

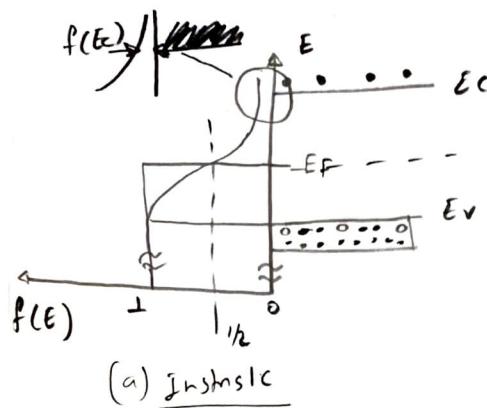
• When $(E > E_F)$
↳ $\frac{1}{1+\infty} = 0$
(exponent positive)

• At $T > 0K$ → some probability exist for states above the Fermi-level.

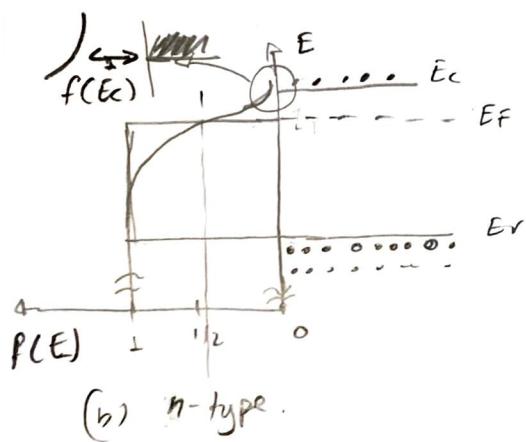
• At $T > 0K$ to be filled.
When $T = T_1$ there is some probability $f(E)$ that states above E_F are filled & there is corresponding probability $1-f(E)$ states below E_F . Fermi-function is symmetrical about E_F for all temperatures.

\therefore The symmetry distribution of empty and filled states about EF makes the Fermi-level a natural reference point in calculations of electron & hole concentration in semiconductors.

- Fermi distribution function applied to semiconductors.

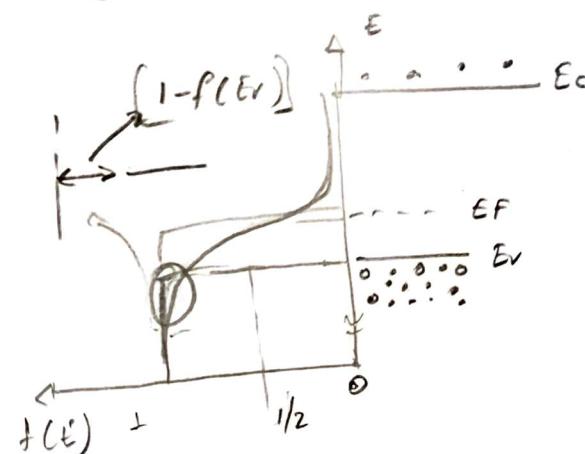


For example: In Si at 300K
 $n_i = p_i = 10^{10} \text{ cm}^{-3}$
 whereas the densities of available states at E_v & E_F are 10^{19} cm^{-3}
 \therefore Probability $[f(E)]$ for an individual state in conduction part (valence band also) is quite small



N-type \rightarrow High concentration of electrons in the conduction band compared to hole concentration in valence band.

Notice that the value of $f(E)$ for each energy level in conduction band $\therefore (n_o) \uparrow$ as E_F moves closer to E_C
 $\therefore (E_C - E_F) \rightarrow$ gives a measure of n



For P-type: Fermi level closer to E_v such that $[1-f(E)]$ tails below E_v is larger than $f(E)$ above E_C .

$\therefore (E_F - E_v) \rightarrow$ gives measure of p

Electron & Hole Concentrations at Equilibrium

→ Fermi distribution can be used to calculate the concentrations of electrons & holes in a semiconductor

$$① \quad n_0 = \int_{E_C}^{\infty} f(E) N(E) dE$$

• $N(E) dE \rightarrow$ density of states (cm^{-3}) in the energy range dE

• Subscript 0 (n_0) \rightarrow indicates equilibrium conditions,

• Note: Proof of $N(E) \rightarrow$ see book

→ $N(E) \propto E^{1/2} \therefore$ density of states in the conduction band ↑ with electron energy ↑

→ $f(E) \downarrow \downarrow \rightarrow$ for large energies

∴ Product $f(E) N(E)$ decreases rapidly above E_C & very few electrons occupy energy states far above the conduction band edge

* Similarly for holes *

[See book pg 87] *

• $N_c \rightarrow$ effective density of states

$$② \quad n_0 = N_c f(E_C)$$

↳ Direct result of integration (1)

• By assuming the Fermi-level (E_F) lies at least several kT below the conduction band

∴ The exponential term is large compared with unity & Fermi function simplifies

$$f(E_C) = \frac{1}{1 + e^{(E_C - E_F)/kT}} \approx e^{-(E_C - E_F)/kT}$$

$$\therefore n_0 = N_c e^{-(E_C - E_F)/kT} \quad ③ //$$

Effective Density of States (N_c)

$$N_c = 2 \left(\frac{2\pi m_n^* kT}{h^2} \right)^{3/2}$$

$\rightarrow m_n^*$ \rightarrow density of states effective mass for electrons

Obtained from the band curvature effective masses

$$\therefore (m_n^*)^{3/2} = 6(m_e m_t)^{1/2} \quad \left. \begin{array}{l} \text{geometric mean of the} \\ \text{effective masses} \end{array} \right\}$$

Concentration of holes in the valence band

$P_0 = N_v [1 - f(E_v)]$ $\cdot N_v \rightarrow$ effective density of states in the valence band

\therefore The probability of finding an empty state at E_v is:

$$1 - f(E_v) = 1 - \frac{1}{1 + e^{(E_v - E_F)/kT}} \approx e^{-(E_F - E_v)/kT}$$

$$\therefore P_0 = N_v e^{-(E_F - E_v)/kT}$$

Effective Density of states in the valence band reduced to the band edge

$$N_v = 2 \left(\frac{2\pi m_p^* kT}{h^2} \right)^{3/2}$$

Predicts that the hole concentration increases as E_F moves closer to the valence band

- For intrinsic material, E_F lies at some intrinsic level E_i near the middle of the band gap.

$$\therefore n_i = N_c e^{-(E_c - E_i)/kT}, p_i = N_v e^{-(E_i - E_v)/kT}$$

- The product $n_0 \times p_0$ at equilibrium is constant for a particular material and temperature, even if the doping is varied.

$$n_0 p_0 = (N_c e^{-(E_c - E_F)/kT}) \cdot (N_v e^{-(E_F - E_v)/kT}) \\ = N_c N_v e^{-(E_c - E_v)/kT} = N_c N_v e^{-E_g/kT}$$

$$n_i p_i = (N_c e^{-(E_c - E_i)/kT}) \cdot (N_v e^{-(E_i - E_v)/kT}) \\ = N_c N_v e^{-E_g/kT}$$

- The intrinsic electron & hole concentrations are equal (since the carriers are created in pairs), $n_i = p_i \therefore$

$$n_i = \sqrt{N_c N_v} e^{-E_g/2kT}$$

$$\therefore (\Rightarrow) \boxed{n_0 p_0 = n_i^2} \quad \textcircled{A}$$

Note:

$$n_0 = n_i e^{(E_F - E_i)/kT}$$

$$p_0 = p_i e^{(E_i - E_F)/kT}$$

} $\left. \begin{array}{l} \cdot n_i \text{ when } E_F \text{ is at the intrinsic level } (E_i) \\ \cdot n_0 \uparrow \text{exponentially as Fermi level moves away from } E_i \text{ toward conduction band} \end{array} \right\}$

Example:

A Si sample is doped with 10^{17} As atoms/cm³. What is the equilibrium hole concentration p_0 at 300K?

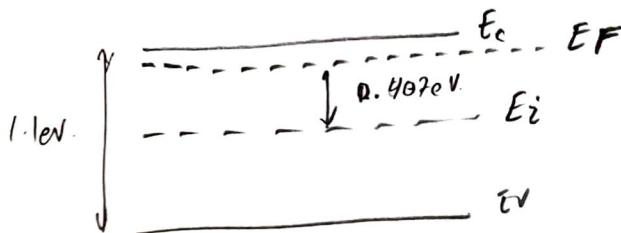
→ Since $N_d \gg n_i$ we can approximate $n_0 = N_d$

$$\therefore p_0 = \frac{n_i^2}{n_0} = \frac{2.25 \times 10^{20}}{10^{17}} = 2.25 \times 10^3 \text{ cm}^{-3}$$

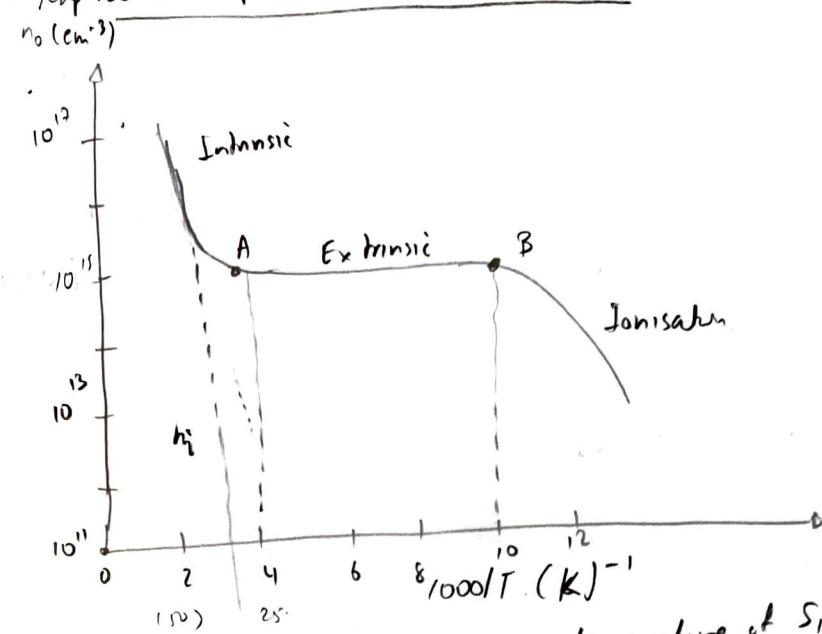
From Equation -

$$n_0 = n_i e^{(E_F - E_i)/kT} \Rightarrow E_F - E_i = 0.407 \text{ eV}$$

(band diagram)



Temperature Dependence of Carrier Concentration



→ Carrier concentration vs inverse temperature of Si doped with 10^{15} donor/cm³

Explanation:

- At low temperatures (large $1/T$), negligible intrinsic EHP exist.
The donor electrons are bound to the donor atoms.
- As $T \uparrow$, electrons are donated to the conduction band and at about $100K$ ($1000/T = 10$) [B] all the donor atoms are ionised.
 \therefore ionisation region.
- Once donors are ionised \therefore conduction band electron concentration $n_0 \approx N_d \approx 10^{15}$ \therefore
- At higher temperatures, n_i is much greater than N_d . The intrinsic carriers dominate.