Elementary Band Theory

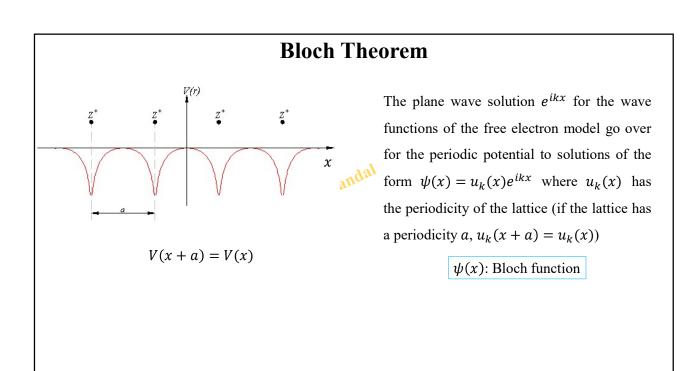
Introduction

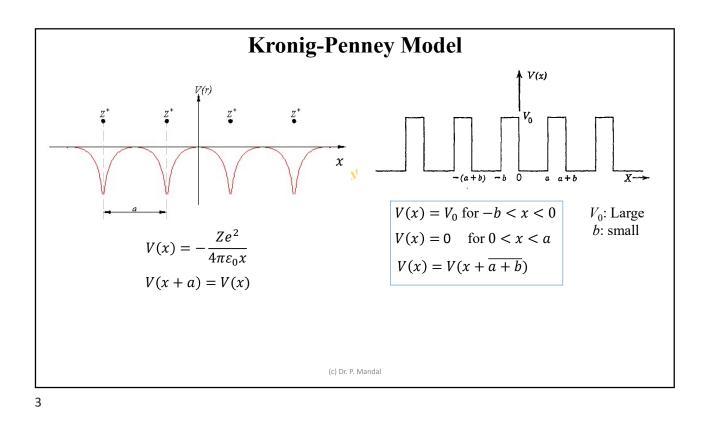
□ How to distinguish between metal and semiconductor/insulator?

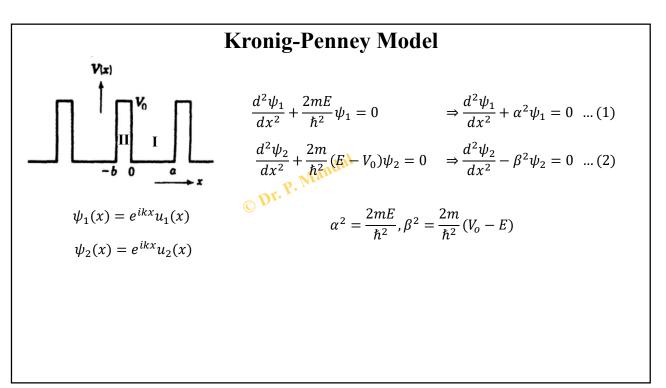
□ What is the origin of positive Hall coefficients?

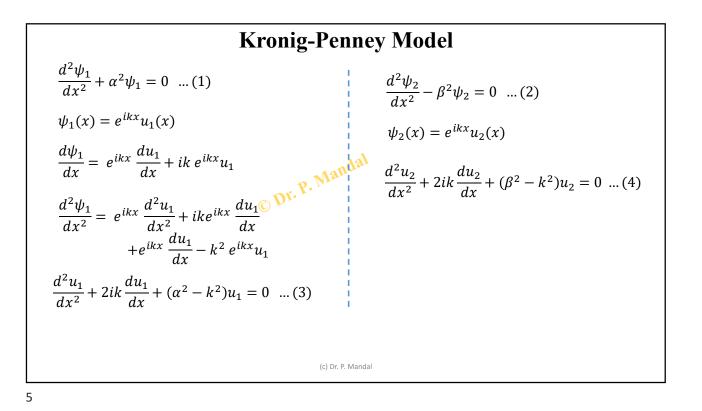
- Use Well, free electron theory of solids does not answer to these questions!
- A productive theory comes from band theory of solids

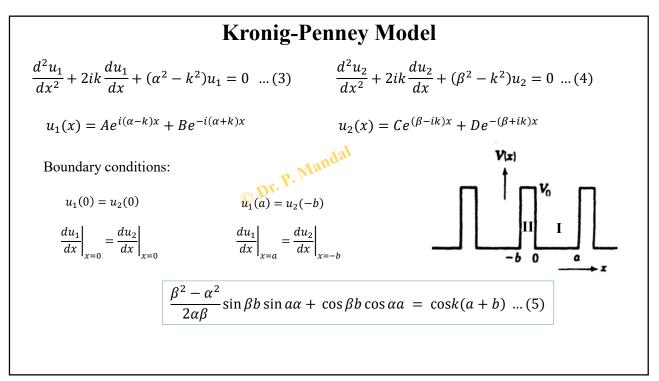
Syllabus: Kronig Penny model. Band Gap. Conductor, Semiconductor (P and N type) and insulator. Conductivity of Semiconductor, mobility, Hall Effect. Measurement of conductivity (4 probe method) & Hall coefficient

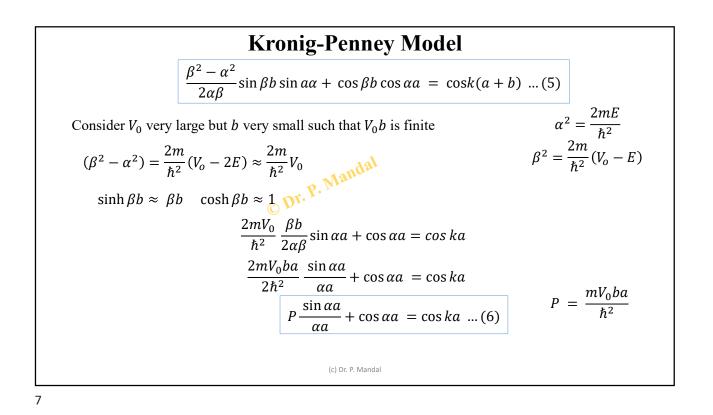


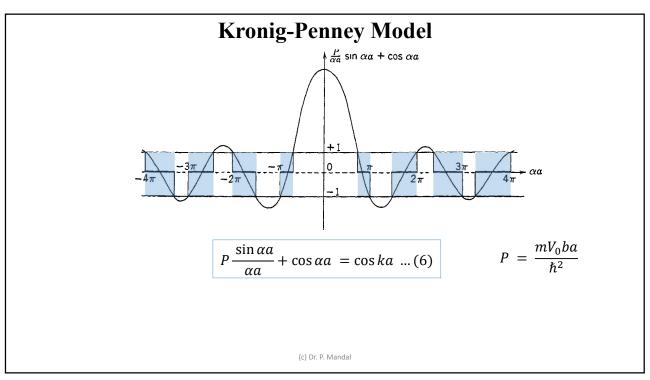


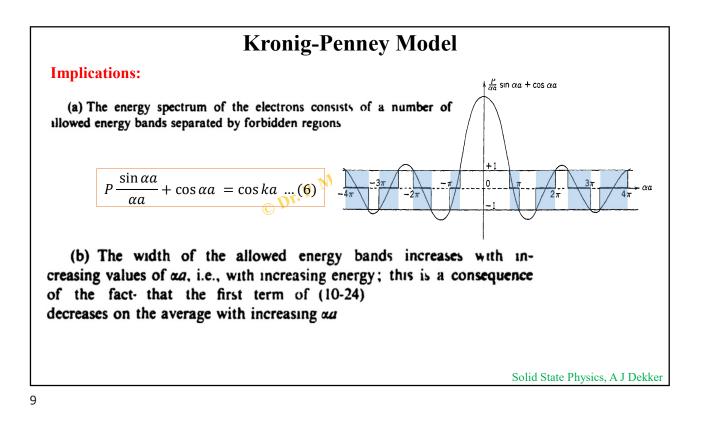


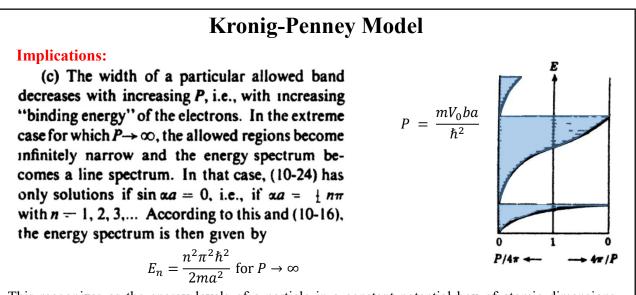












This recognizes as the energy levels of a particle in a constant potential box of atomic dimensions. Physically, this could be expected because for large P, tunneling through the barriers becomes improbable.

Kronig-Penney Model

Implications:

These conclusions are summarized in Fig. 10-3, where the energy spectrum is given as function of P. For P = 0, we simply have the free electron model and the energy spectrum is (quasi) continuous; for $P = \infty$, a line spectrum results as discussed under (c) above. For a given value of P the position and width of the allowed and forbidden bands are obtained by erecting a vertical line; the shaded areas correspond to allowed bands.

From (10-24) it is possible also to obtain the energy E as function of the wave number k; the result is represented in Fig. 10-4a. This leads us to the conclusion that

$$P = \frac{mV_0ba}{\hbar^2}$$



P/4# -

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Kronig-Penney Model

Implications:

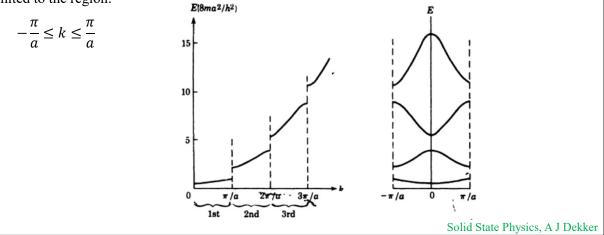
(d) Discontinuities in the E - k curve: $k = \frac{n\pi}{a}$, n = 1, 2, 3, ...

These k-values define the boundaries of the first, second, etc. Brillouin zones. It must be noted that Fig. 10-4a gives only half of the complete E(k) curve; thus the first zone extends from $-\pi/a$ to $+\pi/a$. Similarly, the second zone consists of two parts; one extending from π/a to $2\pi/a$, as shown, and another part extending between $-\pi/a$ and $-2\pi/a$.

Kronig-Penney Model

Implications:

(e) Within a given energy band, the energy is a periodic function of k. For example, if one replaces k by $k + 2\pi n/a$, where n is an integer, $\cos ka$ remains the same. In other words, k is not uniquely determined. It is therefore frequently convenient to introduce the "reduced wave vector" which is limited to the region:



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Kronig-Penney Model

Implications:

(f) Number of possible wave functions per band:

Boundary condition: Cyclic or periodic boundary conditions - same as in the theory of elastic waves

in a chain of atoms: $\psi(x + L) = \psi(x)$ $\Rightarrow e^{ik(x+L)}u_k(x + L) = e^{ikx}u_k(x)$ $\Rightarrow e^{ikL} = 1 = e^{i2n\pi} \Rightarrow k = 2n\pi/L, n = \pm 1, \pm 2, \pm 3, ...$

Number of possible wave functions in the range dk: $dn = (L/2\pi)dk$

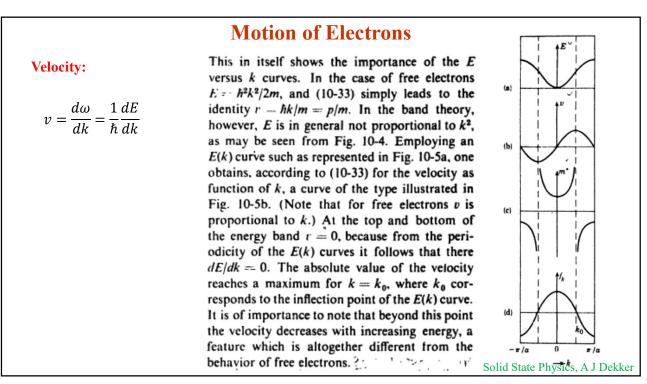
$$n_{max} = \int_{-\pi/a}^{\pi/a} (L/2\pi) dk = \frac{L}{a} = N$$

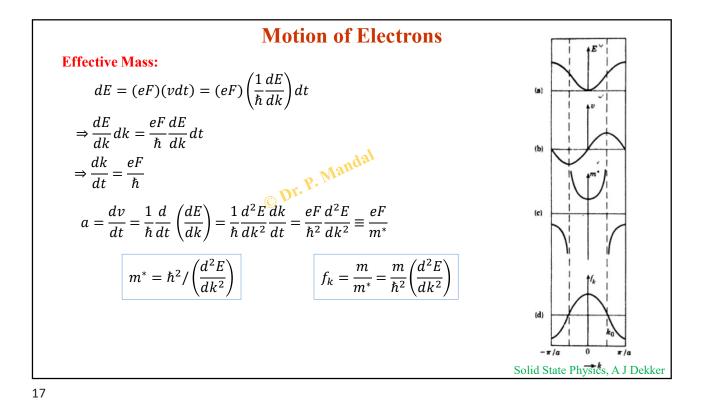
Kronig-Penney Model

Implications:

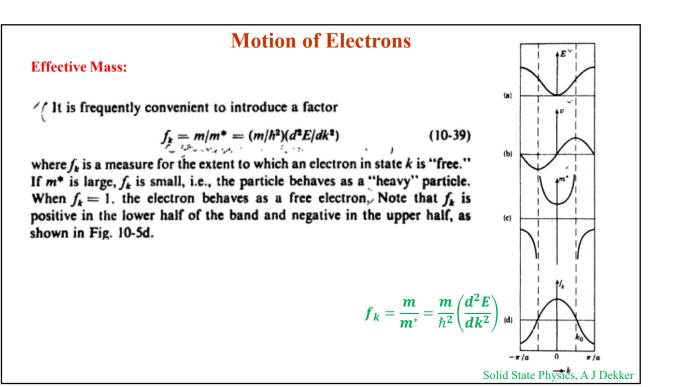
 $\mathcal{A}(f)$ The total number of possible wave functions in any energy band isequal to the number of unit cells N.

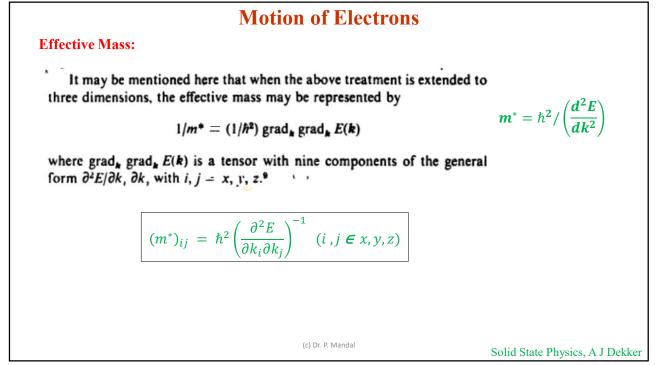
Now, as a result of the spin of the electrons and the Pauli exclusion principle each wave function can be "occupied" by at most two electrons.⁵ Thus each energy band provides place for a maximum number of electrons equal to twice the number of unit cells. In other words, if there are 2N electrons in a band, the band is completely filled. This conclusion, as we shall see below, has far-reaching consequences for the distinction between metals, insulators, and semiconductors.





Motion of Electrons $m^* = \hbar^2 / \left(\frac{d^2 E}{dk^2}\right)$ **Effective Mass:** Thus the effective mass is determined by d^2E/dk^2 ; this result indicates once more the importance of the E(k) curves for the motion of the electrons. In Fig. 10-5c the effective mass is represented as a function of $k \ge 1$ this curve shows the interesting feature that m^* is positive in the lower half of the energy band and negative in the upper half. At the inflection points in the E(k) curves, m^* becomes infinite. Physically speaking, this means that in the upper half of the band the electron behaves as a positively (c) charged particle, as will be explained further in Sec. 10-6. One arrives at the same conclusion by considering the v(k) curve and making use of (10-35). Suppose an electron starts at k = 0; when an electric field is applied, the wave vector increases linearly with time. Until the velocity reaches its maximum value, the electron is accelerated by the field; beyond the maximum, however, the same field produces a decrease in v, i.e., the mass must become negative in the upper part of the band. **π**/a





Motion of Electrons

Effective Mass:

Problem: The dispersion relation of electrons in a 3d lattice is given by $E_k = \alpha \cos k_x a + \beta \cos k_y a + \gamma \cos k_z a$, where *a* is the lattice constant and α, β, γ are constants. Find the effective mass of tensor at the corner of the first Brillouin zone $(\pi/a, \pi/a, \pi/a)$. [CU – 2016]

$$(m^{*})_{ij} = \hbar^{2} \left(\frac{\partial^{2} E}{\partial k_{i} \partial k_{j}} \right)^{-1} (i, j \in x, y, z)$$

$$(m^{*})_{xx} = \hbar^{2} \left(\frac{\partial^{2} E}{\partial k_{x}^{2}} \right)^{-1} \bigg|_{k_{x}=k_{y}=k_{z}=\pi/a} \overset{\text{P. Mandal}}{=} \hbar^{2} (-\alpha a^{2} \cos k_{x} a)^{-1} \bigg|_{k_{x}=\pi/a} = \frac{\hbar^{2}}{\alpha a^{2}}$$

$$(m^{*})_{yy} = \hbar^{2} \left(\frac{\partial^{2} E}{\partial k_{y}^{2}} \right)^{-1} \bigg|_{k_{x}=k_{y}=k_{z}=\pi/a} = \hbar^{2} (-\beta a^{2} \cos k_{y} a)^{-1} \bigg|_{k_{x}=\pi/a} = \frac{\hbar^{2}}{\beta a^{2}}$$

$$(m^{*})_{zz} = \hbar^{2} \left(\frac{\partial^{2} E}{\partial k_{z}^{2}} \right)^{-1} \bigg|_{k_{x}=k_{y}=k_{z}=\pi/a} = \hbar^{2} (-\gamma a^{2} \cos k_{y} a)^{-1} \bigg|_{k_{x}=\pi/a} = \frac{\hbar^{2}}{\gamma a^{2}}$$

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 $\begin{array}{l}
\textbf{Motion of Electrons}\\
\textbf{Effective Mass:}\\
(m^*)_{ij} &= \hbar^2 \left(\frac{\partial^2 E}{\partial k_i \partial k_j} \right)^{-1} (i, j \in x, y, z) \\
(m^*)_{xy} &= \hbar^2 \left(\frac{\partial^2 E}{\partial k_x \partial k_y} \right)^{-1} \bigg|_{k_x = k_y = k_z = \pi/a} = \hbar^2 \left\{ \frac{\partial}{\partial k_x} \left(-\beta a \sin k_y a \right) \right\}^{-1} \bigg|_{k_x = k_y = k_z = \pi/a} = \infty \\
\textbf{Similarly,} \quad (m^*)_{zx} &= (m^*)_{xz} = (m^*)_{zy} = (m^*)_{yz} = (m^*)_{yx} = \infty \\
m^* &= \frac{\hbar^2}{a^2} \begin{pmatrix} 1/\alpha & \infty & \infty \\ \infty & 1/\beta & \infty \\ \infty & \infty & 1/\gamma \end{pmatrix} \quad \text{Or,} \quad \frac{1}{m^*} = \frac{a^2}{\hbar^2} \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \gamma \end{pmatrix}
\end{array}$

Motion of Electrons

Problem: Consider the dispersion relation of tightly bound electrons in a linear lattice with atomic separation a as $E = E_0 - \alpha - 2\gamma \cos ka$ (α, E_0, γ are constants). Obtain an expression of the reciprocal of effective mass (m^*) as a function of E. Sketch $1/m^*$ as a function of E. Also, find the maximum velocity of the electrons. [CU - 2015]

$$E = E_0 - \alpha - 2\gamma \cos ka$$

$$\Rightarrow \frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{1}{\hbar^2} (-2\gamma)(-a)\alpha \cos ka = \frac{2\gamma a^2}{\hbar^2} \cos ka = \frac{a^2}{\hbar^2} (E_0 - \alpha - E)$$

$$v = \frac{1}{\hbar} \frac{dE}{dk} = \frac{1}{\hbar} (2\gamma a \sin ka) \Rightarrow v_{max} = \frac{2\gamma a}{\hbar}$$

$$E_{max} = E\Big|_{k=-\pi/a} = E_0 - \alpha + 2\gamma$$

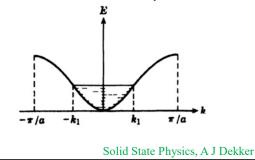
$$E_{min} = E\Big|_{k=0} = E_0 - \alpha - 2\gamma$$
Bandwidth: $E_{max} - E_{max} = 4\gamma$

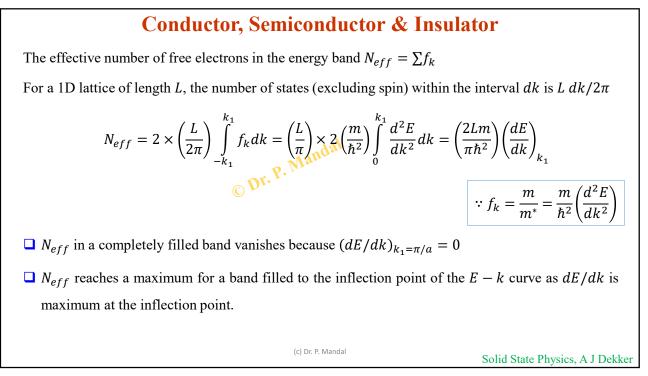
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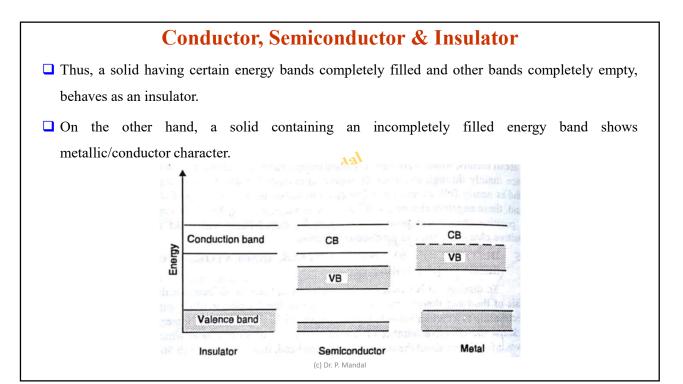
Conductor, Semiconductor & Insulator

- □ Band theory of solids leads to the possibility of distinguishing between conductors, semiconductors and insulators.
- \Box Consider a particular energy band to be filled up with electrons up to a certain value k_1 .
- □ In order to study the effect of an external electric field, we need to know how many electrons are equivalent to 'free electrons' in the band containing certain number (say, N) of electrons.
- The answer to this point, presumably, leads to draw a conclusion on the conductivity associated to this particular energy band.

(c) Dr. P. Mandal







Conductor, Semiconductor & Insulator

Fig. 10-7a can occur actually only at absolute zero, when the crystal is in its lowest energy state. At temperatures different from zero, some electrons from the upper filled band will be excited into the next empty band ("conduction band") and conduction becomes possible. If the forbidden energy gap is of the order of several electron volts, however, the solid will remain an "insulator" for all practical purposes. (An example is diamond, for which the forbidden gap is about 7 ev.) For a small gap width, say about 1 ev, the number of thermally excited electrons may become appreciable and in this case one speaks of an intrinsic semiconductor. Examples are germanium and silicon. It is evident that the distinction between insulators and intrinsic semiconductors at T = 0, whereas all insulators may be considered semiconductors at T > 0. It may be noted here that the conductivity of semiconductors in general increases with increasing temperature, whereas the conductivity of metals decreases

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Concept of Hole

- □ In an intrinsic semiconductor a certain number of electrons are thermally exited from the upper filled band into the conduction band at temperature above 0K, leaving some of the states in the normally filled band vacant. These unoccupied states lie near the top of the filled band.
- Consider a single unoccupied state the 'hole', in the filled band of a 1D lattice and consider its influence on the collective behaviour of this band in presence of an external electric field.
- In absence of external electric field, the current due to all the electrons in a completely filled band

$$I = -e\sum_{i} \vec{v}_i = -e\left[\vec{v}_j + \sum_{i \neq j} \vec{v}_i\right] = 0$$

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Concept of Hole

If the jth electron were missing

 $I' = -e \sum_{i \neq j} \vec{v}_i = e \vec{v}_j$

In presence of an external electric field \vec{F} , the rate of change of the current I' is

As the vacant state ('hole') lies near the top of the band, the effective mass m_j^* is negative which makes dI'/dt positive. In other words, a state in which an electron is missing behaves as a 'positive hole' with an effective mass $|m_i^*|$.

(c) Dr. P. Mandal

Solid State Physics, A J Dekker

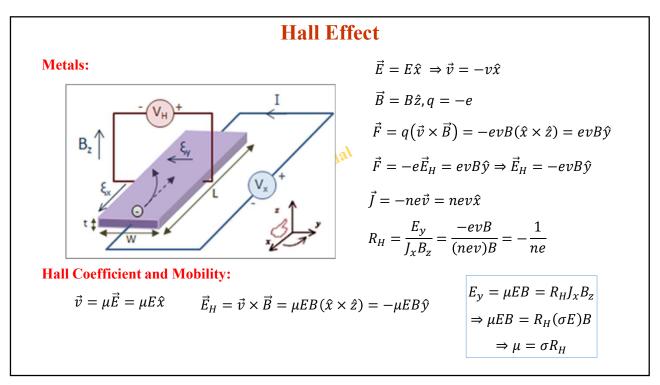
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Hall Effect

- □ The Hall effect is the production of a voltage difference (the Hall voltage V_H) across a conductor or semiconductor, transverse to an electric current (J_x) in the conductor/semiconductor and to an applied magnetic field (B_z) perpendicular to the current.
- Discovered by Edwin Hall in 1879.
- The Hall coefficient is defined as the ratio of the induced electric field to the product of the current density and the applied magnetic field.

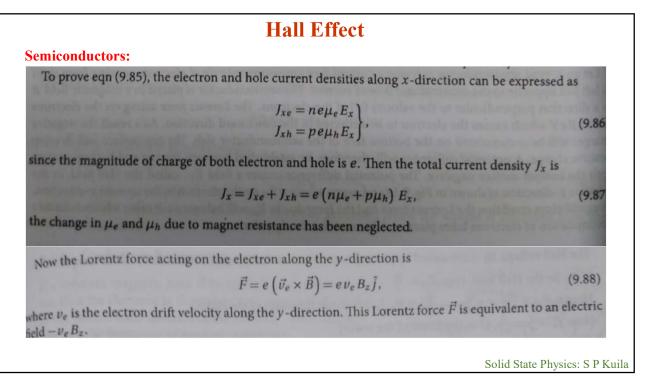
$$R_H = \frac{E_y}{J_x B_z}$$

 \square R_H is the characteristic of the material from which the conductor/semiconductor is made, since its value depends on the type, number, and properties of the charge carriers that constitute the current.

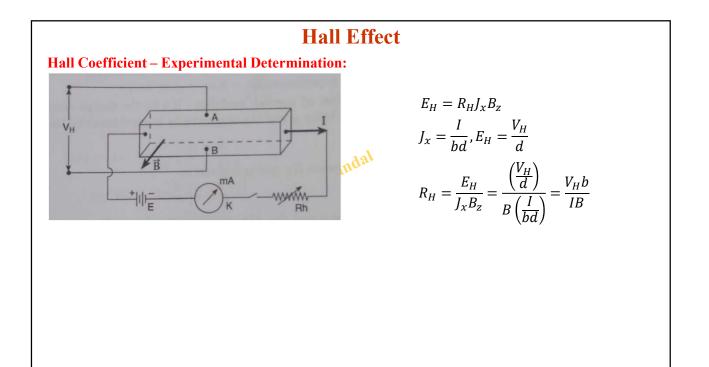


Hall EffectSemiconductors:Since for n-type semiconductor the carriers are negatively charged electrons, $\therefore R_H = -\frac{1}{ne}$.(9.83)For p-type semiconductor the carriers are positively charged. $\therefore R_H = \frac{1}{pe}$,(9.84)Where p is the density of holes. Eqns (9.83) and (9.84) show that the Hall coefficient R_H are of opposite sign for n-type and p-type semiconductors.When the contribution of both the electrons and holes to the current are appreciable, Hall coefficient may be proved to be $R_H = \frac{p\mu_h^2 - n\mu_h^2}{e(n\mu_e + p\mu_h)}$,(9.85)aince $\sigma = ne\mu_e + pe\mu_h$ and μ_e, μ_h are the mobilities of electrons and holes respectively.

Solid State Physics: S P Kuila



Hall Effect Semiconductors:		
nd hole current density J_{yh} along Y-direction is $J_{yh} = p e \mu_p^2 B_z E_x.$	(9.90)	
So, the total current density along <i>Y</i> -direction is $J_y = J_{ye} + J_{yh} = e \left(n\mu_e^2 - p\mu_h^2 \right) B_z E_x.$	(9.91)	
To make the net current density J_y zero a Hall field E_y is required. $\therefore \frac{E_y}{E_x} = \frac{J_y}{J_x} \text{ or, } J_x E_y = J_y E_x \text{ or, } e(n\mu_e + p\mu_h) E_y = -e(n\mu_e^2 - p\mu_h^2) B_z E_x$ $n\mu_e^2 - n\mu_e^2$	and some stars	
or, $E_y = \frac{p\mu_h^2 - n\mu_e^2}{n\mu_e + p\mu_h}B_z E_x.$ The Hall coefficient R_H is given by	(9.92	
$R_{H} = \frac{E_{y}}{B_{z}J_{x}} = \frac{p\mu_{h}^{2} - n\mu_{e}^{2}}{e(n\mu_{e} + p\mu_{h})^{2}}.$	(9.93 Solid State Physics: S P Kuil	



Hall Effect		
Applications:		
are negatively charged e that the semiconductor semiconductor is of p -ty 2. Determination of the electrons can be obta Hall coefficient R_H expe 3. Determination of	of the nature of the semiconductor—If the current carriers lectrons, the measured value of R_H is negative which indicates is an <i>n</i> -type one. If, on the other hand, R_H is positive the pe having holes as majority carriers. of carrier concentration—The concentration of the holes and ained from either (1.16.5) or (1.16.6), provided we measure the rimentally. of carrier mobility—If ρ be the charge density of a semicon- y μ and the conductivity σ are related by the equation	
The Distance state which we are	$\sigma = \rho \mu$.	
The relation between	R_H and μ is given by	
	$\mu = \sigma R_H$	
mobility and is known as	of magnetic field—From (116.12)	
the second of the magne	the held <i>B</i> . $B = \frac{V_H b}{IR_H},$ Solid State Physics: Gupta & Islam	