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B.Sc (PS)Computer Science VI Sem

Kronig Penney model

E Vs. K Diagram:-

The electron moving in a periodic potential lattice can have energy values only between allowed regions. From eq. (24) it is possible to plot the total energy \bar{E} of the electron as a function of wave number K fig 4(a). The right hand side of eq. (20) becomes ± 1 for values of $K = \frac{n\pi}{a}$, where n takes the values $\pm 1, \pm 2, \pm 3$ etc. From fig 4(a), it is observed that discontinuities occur in E Vs K curve for $K = \pm \frac{\pi}{a}, \pm \frac{2\pi}{a}, \pm \frac{3\pi}{a}$ etc. i.e., the electron energy increases continuously from zero till the value of K reaches $\frac{\pi}{a}$ or $-\frac{\pi}{a}$ and then electron meets a wall and is reflected. The electron has allowed energy region from K values $-\frac{\pi}{a}$ to $\frac{\pi}{a}$ and the zone is called first Brillouin zone. Similarly second zone consists of two parts one extending from $\frac{\pi}{a}$ to $\frac{2\pi}{a}$ and other from $-\frac{\pi}{a}$ to $-\frac{2\pi}{a}$.

These zone boundaries represent the maximum energies that the electron can have without developing any discontinuity. The energy gap at the zone boundaries is called the forbidden gap or band gap. The dotted curve is for large energies i.e. \bar{E} approaches the free electron value given as $E = \frac{\hbar^2 K^2}{2m}$.

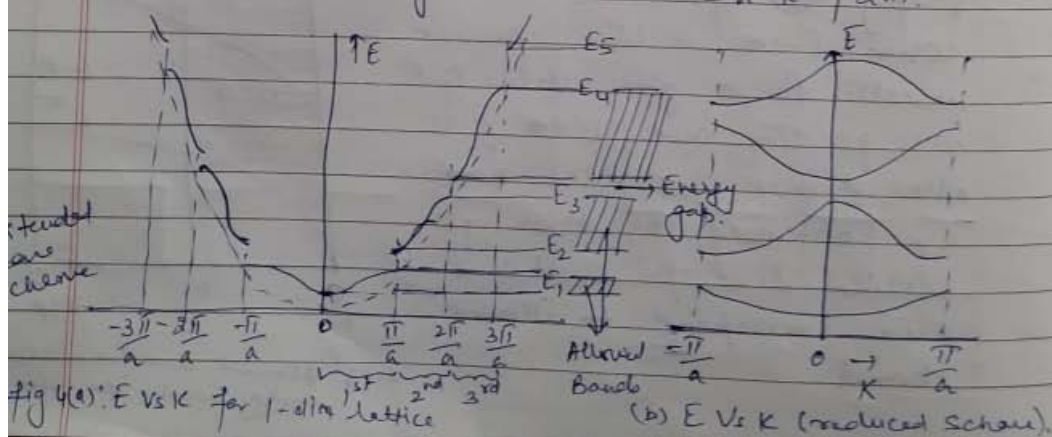


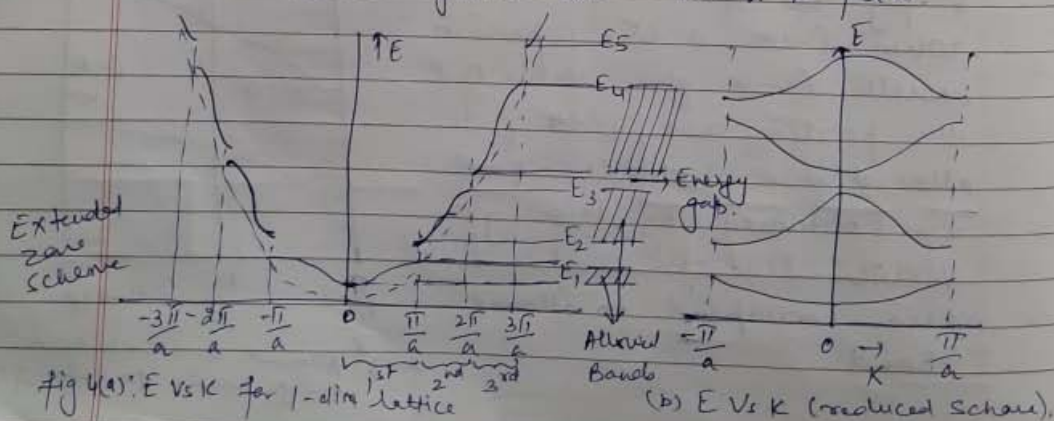
fig 4(a): E Vs K for 1-dim lattice

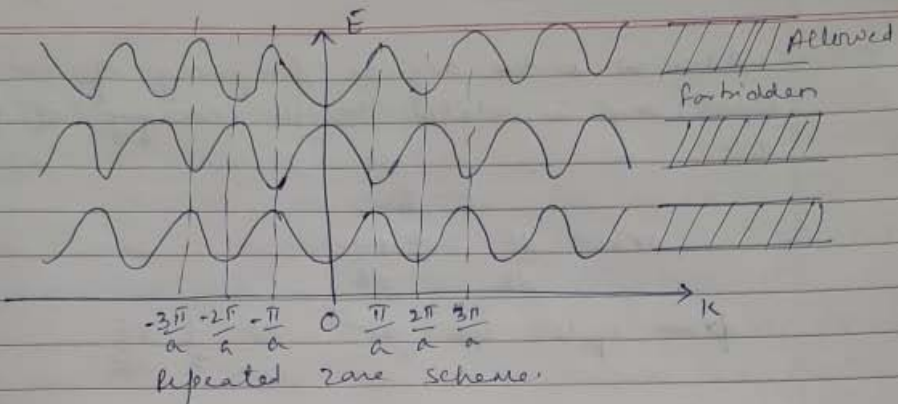
(b) E Vs K (reduced scheme).

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~~velocity~~ The main point to be noticed is that in a 'constant potential' lattice, the electron energy values are same but continuous while in a periodic potential lattice, the electron energy values are discontinuous, separated into allowed and forbidden bands occurring alternately.

Velocity, effective mass and Crystal momentum:

Motion of electron under Kronig-Penney model was considered and expressions for velocity, mass of electron and Crystal momentum were found as follows:

(a) Velocity:- It is well known that an electron has well defined mass and obeys Newton's law when acc. by an electric field. But when the electron is acc. inside the crystal under the electric field, the mass of e^- in the crystal appears different from the free electron mass.

According to de-Broglie, an electron moving with velocity v is considered as a wave packet with group velocity v_g , which is equal to the particle velocity. Thus

$$v_g = v = \frac{d\omega}{dk} \quad (2.8)$$

where ω is the angular frequency of the de-Broglie wave, and is related to the energy of the particle as

$$E = \hbar\omega$$

$$\text{or } \frac{dE}{dk} = \hbar \frac{d\omega}{dk}$$

$$\text{from eq. (28) we get } v = \frac{1}{\hbar} \frac{dE}{dk} \quad (29)$$

where k is the wave number. Now for free e^-

$$E = \hbar^2 k^2 / 2m$$

$$dE/dk = \hbar^2 k / m$$

Putting this value in eq. (29), we get

$$v = \hbar k / m = p/m$$

which gives the linear variation of v with k .

But according to band theory (with periodic potential) of electrons, E is not, in general, proportional to k^2 , therefore the variation of E with k is as shown in fig 5(a). Using this type of variation of E with k and from eq. (29), the velocity v can be calculated. The variation of this velocity as a function of k is shown in fig 5(b).

It is observed that velocity of the electron varies with the slope. For $k=0$ and $k=\pi$, the slope dE/dk is zero. In this way the velocity of the electron is zero at the bottom as well as at the top of the first Brillouin Zone. At intermediate regions in the zone the velocity of the electron reaches the free electron velocity. The absolute value of the velocity reaches a maximum for $k=k_0$, where k_0 corresponds to the inflection point of the $E(k)$ curve. Beyond this point the velocity decreases, with increasing energy, which is quite different from the free electrons behaviour.

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The negative value of the wave number exhibit a similar behaviour.

(b) Effective mass of electron:-

Suppose the electron is initially in a state k and an external electric field \mathcal{E} is applied. Suppose that this is the only electron in the k -z under consideration, so that Pauli exclusion principle does not enter in the discussion. When the electric field \mathcal{E} has acted on the electron for a small time dt , it has gained a velocity v over a distance dx . Thus an increase in energy dE of the electron is given as

$$dE = e\mathcal{E}dx = e\mathcal{E}vdt$$

Putting the value of v from eq. (29) we get

$$dE = \frac{e\mathcal{E}}{\hbar} \left(\frac{dE}{dk} \right) dt$$

$$\text{But } dE = \frac{dE}{dk} dk$$

$$\text{which gives } \frac{dE}{dk} \cdot dk = \frac{e\mathcal{E}}{\hbar} \left(\frac{dE}{dk} \right) dt$$

$$\text{or } \frac{dk}{dt} = \frac{e\mathcal{E}}{\hbar} \quad \text{--- (30)}$$

$$\text{or } \hbar \frac{dk}{dt} = \frac{dp}{dt} = F = e\mathcal{E} \quad \text{--- (31)}$$

where p now denotes the crystal momentum. This equation simply states that rate of change of crystal momentum is equal to the force $e\mathcal{E}$. It is thus an analogue of Newton's law for the electron in a periodic lattice. If ' a ' be the acceleration of the electron, then

$$'a' = \frac{dv}{dt} \text{ and from eq. (29) we get}$$

$$a = \frac{d}{dt} \left(\frac{1}{\hbar} \frac{dE}{dk} \right)$$

$$\text{or } \frac{dv}{dt} = \frac{1}{\hbar} \frac{d^2E}{dk^2} \cdot \frac{dk}{dt}$$

$$\text{from eq. (30)} \quad \frac{dk}{dt} = \frac{e\mathcal{E}}{\hbar}$$

$$\therefore \frac{dv}{dt} = a = \frac{e\mathcal{E}}{\hbar^2} \frac{d^2E}{dk^2} \quad (32)$$

This shows that the acc. depends upon the value d^2E/dk^2 and is numerically maximum at the B.Z. boundaries.

For the free electrons, we have

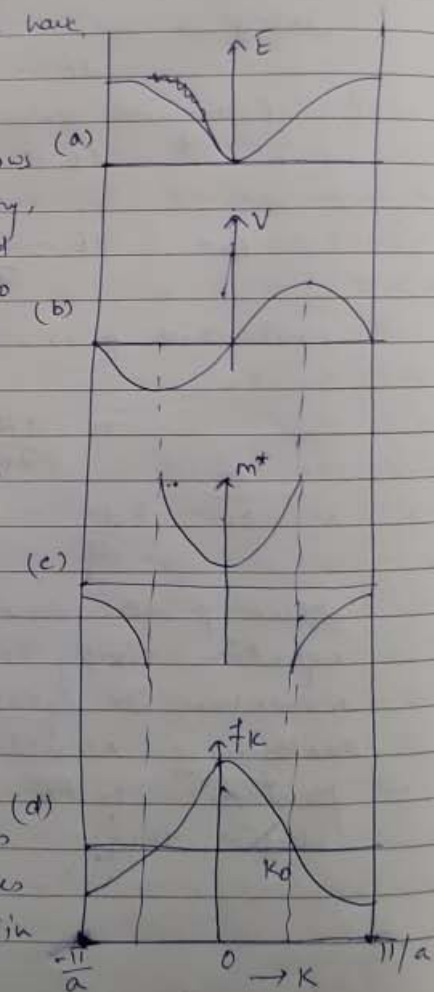
$$a = \frac{e\mathcal{E}}{m} \quad (33)$$

Comparing eq. (32) & (33), it follows that on the basis of band theory, electron behaves as if it had an effective mass m^* equal to

$$m^* = \frac{\hbar^2}{d^2E/dk^2} \quad (34)$$

Thus the effective mass is determined by d^2E/dk^2 and is a function of k . It again indicates the importance of $E(k)$ curve for the motion of the e^- 's. In fig 5(c), the effective mass is rep. as a fun. of k . This fig. shows

fig. 5: Energy, velocity, effective mass and $\hbar k$ as a fun. k . The dashed lines corresponds to the inflection points in the $E(k)$ curve.



that m^* is positive at the bottom of energy band (i.e., in the upper half). At the inflection points in $E(k)$ curve, m^* becomes infinite. Physically speaking the electron behaves as a positively charged particle in the upper half of the band.

Sometimes it is convenient to introduce a

$$f_k = \frac{m}{m^*} = \frac{m}{\hbar^2} \left(\frac{d^2 E}{dk^2} \right) \quad \text{--- (35) factor}$$

where f_k determines the extent upto which the electron in k -state is a free electron. If m^* is large, f_k is small i.e., particles behaves as a heavy particle. When $f_k = 1$, the electron behaves as a free electron, (fig 5(d)).

The negative effective mass may be interpreted in terms of the Bragg reflection when k is close to $\frac{\pi}{a}$, $\frac{2\pi}{a}$ etc. on account of which a force in one direction, because of reflection, leads to a gain of momentum in the opposite direction.

It can be shown that for a free electron $m^* = m$, because

$$E = \frac{\hbar^2 k^2}{2m}$$

$$\text{and } \frac{d^2 E}{dk^2} = \frac{\hbar^2}{m}$$

but for an electron moving in periodic potential, E does not vary with k in the above manner and so $m^* \neq m$. It may be concluded that all the results of the free electron theory are correct provided m in each case is replaced by suitable m^* . Thus

$$E = \frac{\hbar^2 k^2}{2m^*}$$

This is known as the 'effective mass approximation'.

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(c) Crystal momentum:- For a free electron, the quantity $\hbar k$ represents the true momentum of the electron.

It can be seen from

$$E = \hbar^2 k^2 / 2m = \frac{1}{2m} \left(\frac{h^2}{4\pi^2} \right) \left(\frac{4\pi^2}{\lambda^2} \right) \quad \text{as } k = \frac{2\pi}{\lambda}$$

$$\text{or } E = \frac{1}{2m} \frac{h^2}{\lambda^2} = \frac{p^2}{2m} \quad (36)$$

We can understand the dynamical behaviour of free electrons with respect to the true momentum. This is because, there the energy does not vary with k in the way as it does for free electron. Hence the vector $\hbar k$ is termed as crystal momentum and denoted by

$$p_c = \hbar k$$

It is the quantity with respect to which we study the dynamical behaviour of the electron in a periodic potential.

Concept of Holes:-

The negative effective mass m^* occurs for $k > k_0$, where k_0 corresponds to the inflection point of $E-k$ curve, fig 5(a). In other words, it appears only near the top of the energy bands. Thus for materials with nearly filled bands, there will be certain electrons populating the states at the top of the band and will have negative mass m^* . These electrons are of significance because the observable properties of such materials are determined only by these electrons as they lie near the Fermi surface.

Thus consider a band with all states filled except at the top. If an electric field is applied, a group of electrons would shift to this empty state and produce an empty state some where in the interior of the band. The depth of this empty state would depend on the strength of the field. This effect is equivalent to as if one electron has moved from some where in the filled portion of the band to the top and empty state has moved from the top to the interior, through a group of electrons has caused this effect. This empty state is called a hole.

The properties assigned to the holes are:

- (i) The effective mass of a hole is opposite to the effective mass of an electron at the same point in the energy band i.e. $m_h^* = -m^*$
- (ii) The energy of the hole is opposite in sign to the energy of the missing electron i.e., energy of the hole is positive.
- (iii) The drift velocities of the electrons and holes are in opposite direction, but their electric currents are in the same direction which is the direction of the applied electric field.

Fermi Energy and Fermi-level:-

If n and m_s are quantum numbers of an electron in a conduction state, then for a given value of n , there are two possible orientation of an electron spin with $m_s = \pm 1/2$. Suppose we start filling the levels from the bottom ($n=1$) and continue filling the higher levels with electrons

until all N electrons are accommodated. Let n_p denote the top filled energy level. Assuming N to be even, we have $2n_p = N$ which determines the value of n for the upper most filled level.

* At absolute zero all the levels below a certain level will be filled with electrons and all the levels above it will be empty. The level which divides the filled and vacant levels is called Fermi level at absolute zero. The energy of the top most-filled level at absolute zero is called Fermi energy.

Energy bands in solids:- However, with a limited number of electrons in the atom of a solid, it is expected that only the lower energy bands that is completely filled or partially filled is called the valence band in solids. The band that is above the valence band and is empty at 0K, is called the conduction band. The energy region separating the highest occupied band (valence band) from the empty band (conduction band) is termed as forbidden gaps, or energy gap or band gap. These energy gaps are of decisive significance in determining whether a solid is an insulator or a conductor. On the basis of energy band diagram, we shall distinguish between metals, insulators and semi-conductors.

Metals, Insulators and Semi-conductors

For a qualitative between metals, insulators and semi-conductors, let us consider a particular energy band which is assumed to be filled with electrons upto a certain value k , but less than $\frac{\pi}{a}$.

fig (a) : As far as the influence of an external electric field is concerned, one is interested to know as to how many of free electrons are effective. To find the number of effective electrons, we rewrite the factor

$$f_{k_1} = \frac{m}{m^*} = \frac{m}{\hbar^2} \frac{d^2 E}{dk^2}$$

which is a measure for the extent to which an electron in a state k is free to take part in electrical conduction. The effective number of free electrons in a band is equal to

$$N_{\text{eff}} = \sum f_{k_1}$$

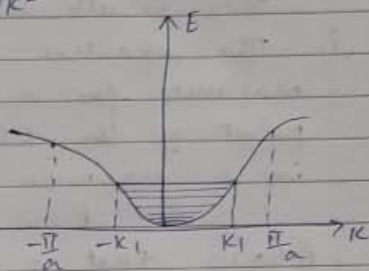


fig (a) : Energy band filled upto state k_1 at $T=0$.

(1)

where the summation extends over all occupied states in the band. In a one dimensional lattice of length L the number of states in the interval dk (excluding the spin) is

$$dn = \frac{L}{2\pi} dk \quad (2)$$

The effective number of conduction electrons within a filled band from limits $-k_1$ to $+k_1$, is given as

$$N_{\text{eff}} = \frac{L}{2\pi} \int_{-k_1}^{k_1} f_{k_1} dk \quad (3)$$

As two electrons occupy each of these states, the term on the right hand is multiplied by 2. Hence

$$N_{\text{eff}} = \frac{2L}{2\pi} \int_{-k_1}^{k_1} f_{k_1} dk = \frac{L}{\pi} \int_{-k_1}^{k_1} f_{k_1} dk$$

Putting the value of f_{k_1} and changing limits to $0 \rightarrow k_1$, we get the effective number of electron

in the band

$$N_{\text{eff}} = \frac{2L}{\pi} \frac{m}{\hbar^2} \int_0^{k_1} \frac{d^2 E}{dk^2} dk$$

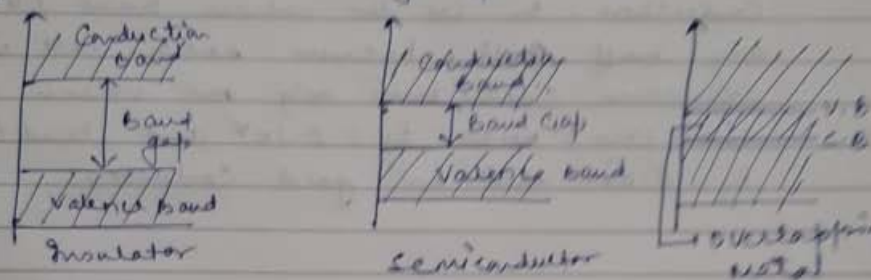
$$\text{or } N_{\text{eff}} = \frac{2mL}{\pi \hbar^2} \left(\frac{dE}{dk} \right)_{k=k_1} \quad (4)$$

This result tells us:

- (i) The effective number of electrons reaches a maximum for a band filled to the inflection point of the $E(k)$ curve, because there dE/dk is a maximum.

From the above discussion, it follows that a solid for which a certain number of energy bands are completely filled, the other bands being completely empty, is an insulator (fig. 6). In other words when there are no effective free electrons, all the bands upto valence band are full and the topmost band called the conduction band is completely empty. This situation shown in fig. (b) can occur actually only at absolute zero, when the crystal is in its lowest energy state. At temperatures different from 0K, some e^- from the upper filled band will be excited into the next empty band (conduction band) and conduction becomes possible. If the forbidden energy region is much wider then solid is an insulator. An example is diamond where the covalent band splits $2s$ and $2p$ levels into two bands separated by an energy gap E_g of about 7eV, with valence electron filling the lower band. When an electric field is applied to such a crystal, there is

no significant change in the state of the valence electrons since a transition to an available level requires an energy which is at least equal to the energy gap. Diamond with $E_g = 7\text{ eV}$, Boron nitride with $E_g = 14.6\text{ eV}$ and Al_2O_3 with $E_g = 7\text{ eV}$ are some e.g. of insulators.



fig(b): Energy band model of insulator, semiconductor and metal -

If the energy gap b/w full and empty band is quite small then there is some probability that the electrons will be excited from states near the top of filled band across the gap to states near the bottom of the empty band. These electrons can conduct electric current and a material of this type is called semi-conductor fig (b). The forbidden gap of semi-conductor, like silicon is about 1 eV . The electrical conductivity of a semiconductor is much smaller and is a function of forbidden energy. Germanium with $E_g = 0.7\text{ eV}$, GaAs ($E_g = 1.43\text{ eV}$) and Indium Antimonide ($E_g = 0.17\text{ eV}$)

If the material has incompletely filled v.b., then there are ~~some~~ enough no. of e^- available for conduction, i.e., they can behave as free

electrons and serve as charge carriers. In terms of energy bands, there will be an overlapping of valence and conduction bands, fig 6 (3rd diagram). Such materials are good conductors of electricity and are called metals. Alkali metals like Na, K, Li and noble metals as Cu, Ag, Au are good conductors. In Cu the valence band (4s band) is only half full, because each cell in f.c.c structure contributes only one valence e⁻s. Metals, tin (grey) with $E_g = 0.1 \text{ eV}$ and lead (Pb) with $E_g = 0.0 \text{ eV}$ act as good conductors.

