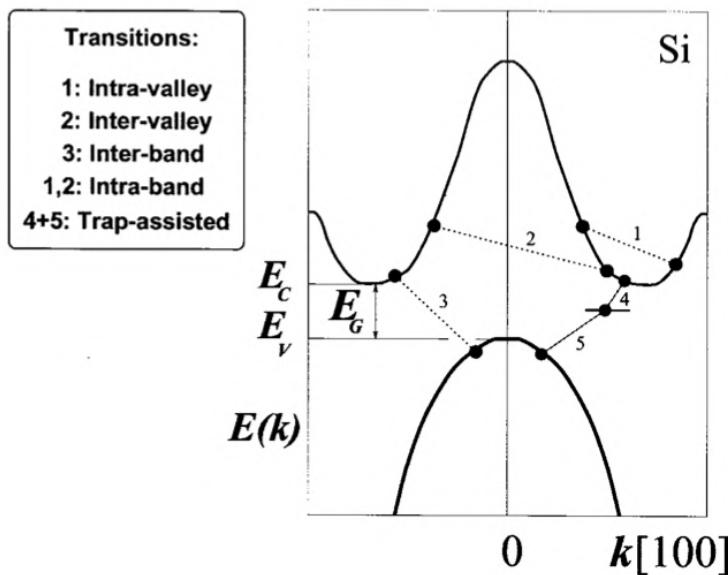


Lecture-3

ఒం శ్రీ ద్వారా గొప్పక్షయ నుంచి



T. 21.15: Due rami delle bande del silicio nella direzione [100].

→ This is the figure describing some of the Energy bands of the silicon which we learned in last class.

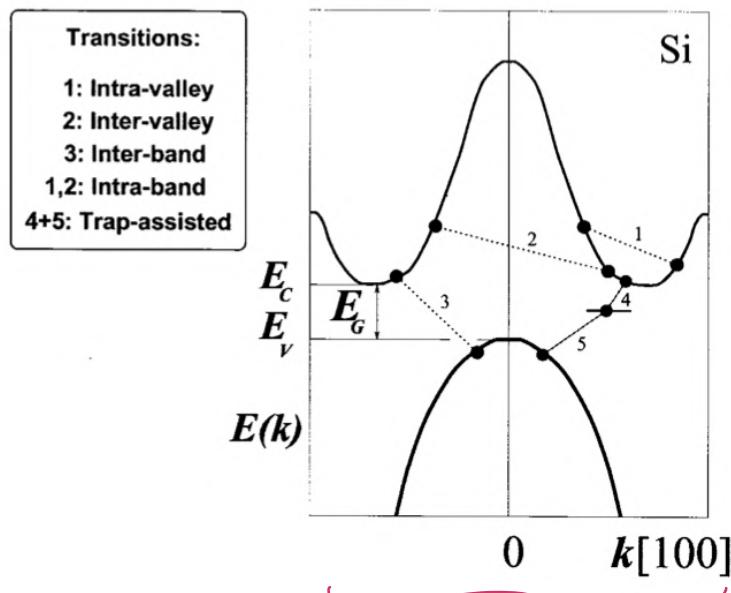
The relation b/w Energy and Avg. Momentum we indicated that

$$\text{Avg. Momentum } (\underline{P}) \propto \text{ } \overset{\circ}{K} \text{ vector}$$

∴ It is customary to use ' $\overset{\circ}{K}$ ' vector instead of Avg. momentum P to describe energy

. ↳

and the Relation b/w Energy & \mathbf{P}
 becomes relation b/w Energy & \mathbf{k}'
 In a crystal ' $\mathbf{k}'' is periodic so it's sufficient
 to consider it within one period and
 this one period is Brillouin Zone
 for Reciprocal Scaled Lattice.$



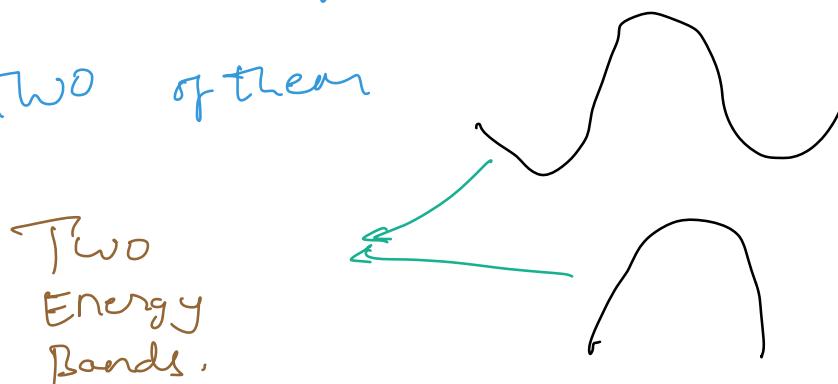
T. 21.15: Due rami delle bande del silicio nella direzione [100].

So the interval for Horizontal axis in the figure is the portion of "Brillouin zone" that for instance of silicon is the two ~~points~~ i.e. two extreme of the interval of the

Horizontal axis are the 'x' points.

→ 'K' vector as we can see in the above figure coincides with $K[100]$ which is the first axis K_1 .

→ The other property of Band structure is there are infinite Bands we see only Two of them



→ But we must imagine that above upper band in the figure there are Infinite other Branches. and Below Lower branch there are other branches but not Infinite.

→ So in principle this structure applies to all electrons of the crystal and each electron has some momentum 'K' and some Energy i.e one of the Branches

\therefore Every electron belongs to a point on one of the Curves (Energy Bands) that corresponds to ' k '

\rightarrow There is still one more property of ' k ' we remember that at some point we started considering Infinite crystal because actual periodicity is present if the structure is Infinitely extended in all directions.

\rightarrow At some point we said this offcourse not true physically. Crystals are finite blocks of matter.

\rightarrow  So how do we extract a Finite Block ?
we simply imagine to start from an Infinite Block of material and cut this Block along parallel plane.
At this point periodicity is lost because

..... - j - - p - - - - - , - - - - -

Finite piece of Block is not periodic anymore

* But, we invented a Trick to Restore
periodicity for a finite Block of Crystal
we fold ^{The} crystal onto itself that
means the left phase of the crystal
is equivalent to the Right phase.

^{ee} Top phase \Rightarrow Bottom phase

^{ee} Front phase \Rightarrow Back face

So, we said this Trick has a Name
it is called Periodic Boundary Condition

→ This Trick has a consequence and
its vector F is not continuous
anymore and it becomes discrete.

Q What does it mean by " F "

is not continuous and becomes

discrete ?

It means that 3 components K_1, K_2, K_3 of vector ' \mathbf{F} ' which we imagined until now as continuous variables are actually countable. i.e. they become functions of Integer Index.

So, you must imagine that each component of ' \mathbf{F} ' is discretized.

for instance $K[100]$ is discretized it depends on an integer index and each possible value of each component of ' \mathbf{F} ' are equally spaced along corresponding axis. Now we must imagine that, we have many possible values of ' \mathbf{F} ' on the axis equally spaced.

This is not terrible constraint, because we can calculate how many possible vector $\underline{\mathbf{F}}$ after discretization takes place

are present inside the Brillouin zone.

→ And it turns out the total no. of distinct or different ' k ' vectors in the Brillouin zone is equal to Total no. of cells in the direct lattice. N_c

N_c is quite large.

$1\text{cm}^3 \rightarrow \text{No. of atoms is } 5 \times 10^{22}$
silicon

This no. of ' k ' vectors in the Brillouin zone.

So, the ' k ' vector is discrete but are very dense. which means that if at some point we need to calculate derivative of Energy wrt ' k ' we can do it as if the ' k ' vector was continuous.

→ For a given ' k ' vector an Electron belongs

in principle to the Infinite Branches.

of Energy and investigate what electrons are doing in each branch. and it wouldn't be feasible.

→ But, we are interested in the behaviour of the electrons because we want to describe the Transport properties of the material.

How the material behaves after being put in Non Equilibrium conditions (Applying external Voltage).

How electric current is flowing through the material and it's carried by electrons.

→ Now some of the Energy bands have no Electrons . i-e if we go up the energy levels that are shown in the picture, we will find branches with High Energy and not electrons generally occupies the High Energy Bands.

- can contain holes.

→ If we start from Equilibrium condition the total energy of the crystal is finite - so it's impossible for the electrons to acquire that is Too High - Because the $T-E$ that can be possessed by the Electrons is Finite.

This is also true of Non-Equilibrium condition.

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∴ High Energy Bands do not give any contribution to the currents in Non Equilibrium condition.

→ On the other hand that have low energy the Bands that are below the lower Band

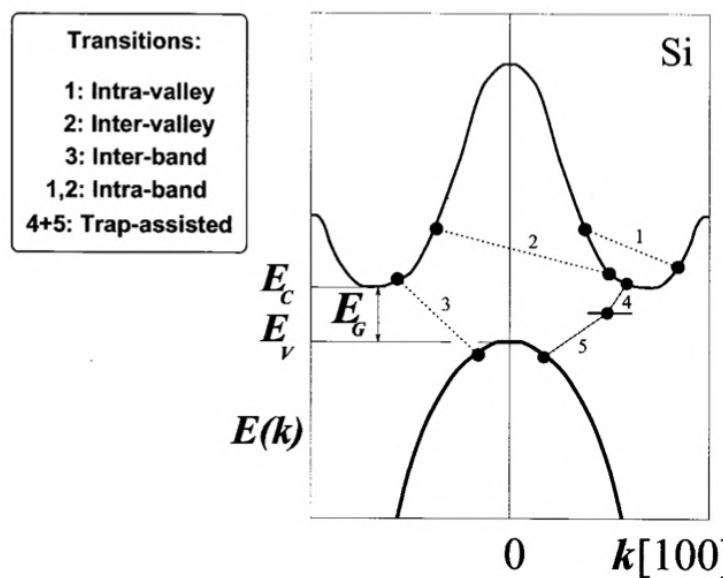


Figure - These ^{lower} bands are completely filled with electrons i.e to each ' k ' vector of

the lower Band there corresponds an Energy and there is one electron possessed in that energy.

- Vector ' k ' is also called a State ∵ each state has an Electron.
- when we have a Band i.e. completely filled with electrons i.e. each ' k ' and each "Energy of the Band" has electrons in it.
- This completely filled Band will not be able to contribute to electric current. This looks Quite odd !
- ∵ High Energy Bands }
completely filled Bands } → Do not contribute current.

Conclusion:- Only Partially Filled bands contribute to Electric current.



T. 21.15: Due rami delle bande del silicio nella direzione [100].

The two partially filled Bands are shown in the figure.

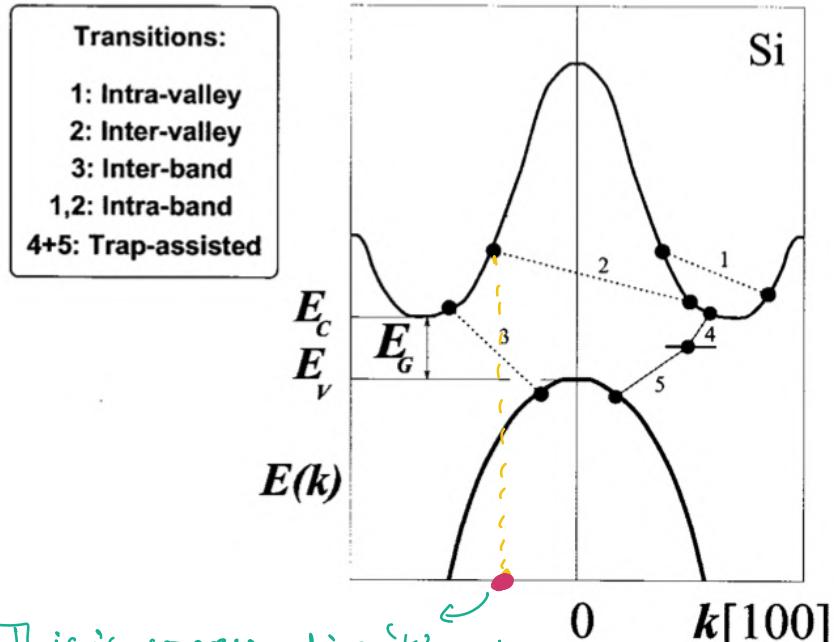
These two special Bands :- have special place.

The Upper Band \rightarrow Conduction Band

Lower Band \rightarrow valance Band.

\rightarrow The '•' Black dots represent

Electrons



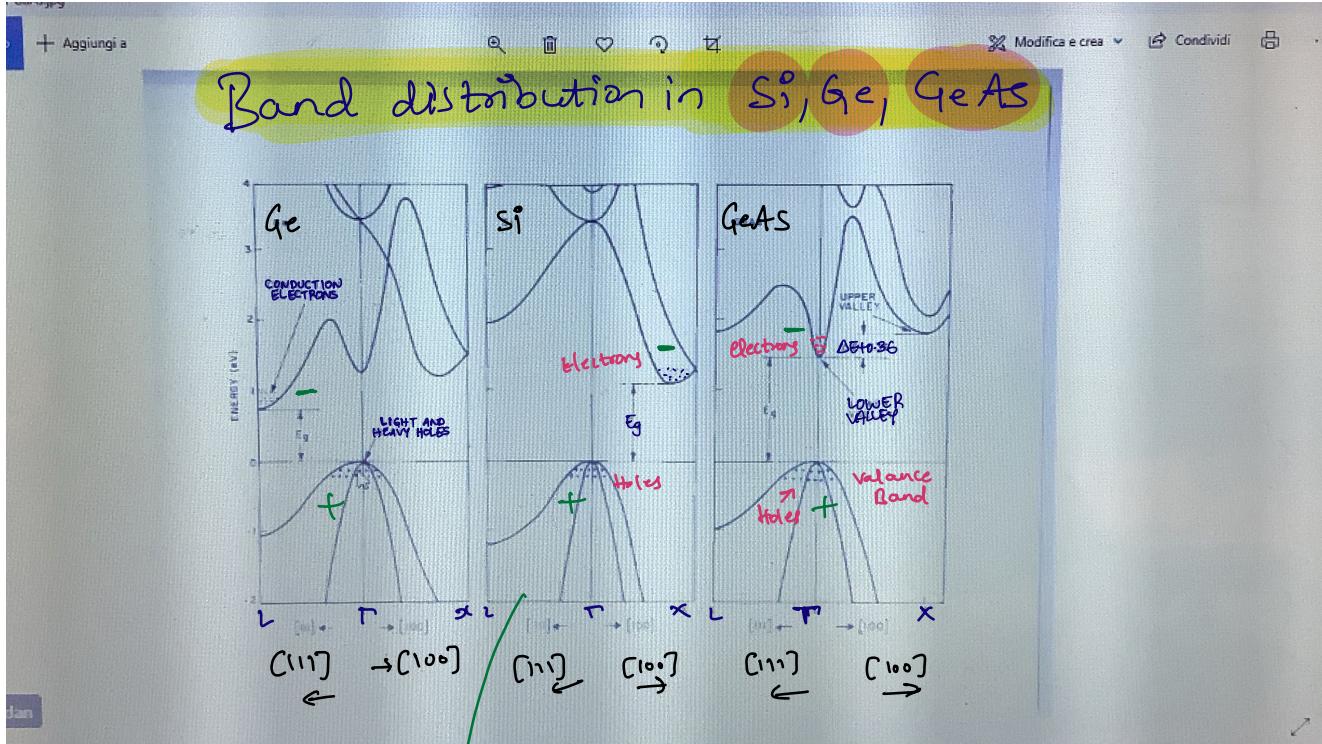
This is corresponding 'k' vector
for the electron

→ 'k' is on horizontal and corresponding
Energy is on vertical axis

→ If electron is subjected to external
perturbation.

→ Soothing
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T. 21.15: Due rami delle bande del silicio nella direzione [100].



Here two Branches (i.e. Bands) have same maximum energy. The curvature is different.

→ This means that electronic states of the valence bands are not occupied by electrons near the maxima. So it's deal w.r.t. symbol w.r.t. conduction band. It has holes.

→ $[100]$ goes from Γ to X
 $[111]$ goes from Γ to L

If we see in germanium the absolute

minimum in conduction band is along the [111] direction and precisely it is at L point.

The total no. of 'L' points in a crystal like Si & Ge is '8'.

→ So Germanium has '8' minimum in the conduction. However the minimum is exactly at the boundary of the Brillouin zone. That means $\frac{1}{2}$ of the minimum is inside Brillouin zone and the other half is outside.

→ So the total minima of the conduction band is '4' not '8' because we should count the part that is only inside the Brillouin zone.

→  It means that the particle the belongs to one of the two branches in the valence band has effective Mass.

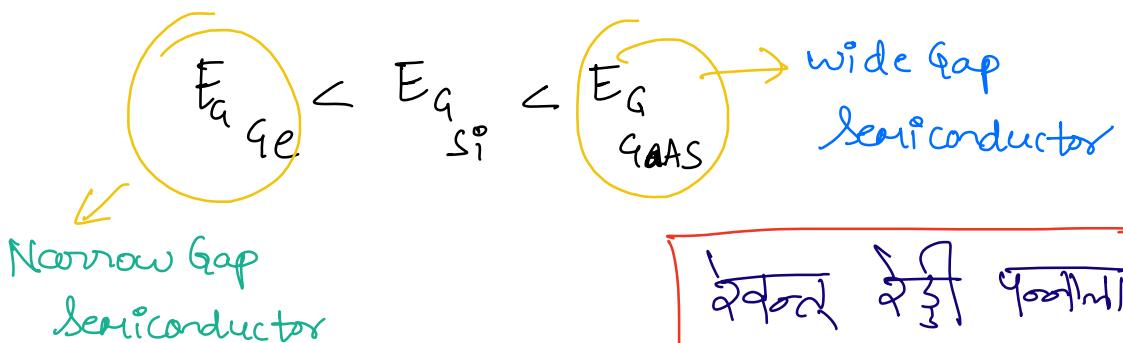
that's diff. from another.
we will discuss this in other occasion.

→ In Gats

It has a valence band whose structure is same compared to Si and Ge it has two branches with same values of the maximum.

→ Instead there is only Minimum in the conduction band and this minimum corresponds to $T(\text{gamma})$ point.

→ let's now consider about the Energy Gap.
gap b/w
i.e Maximum of Valence Band to Minimum of conduction Band.



→ If we consider silicon and Germanium we see that Maxima of valence band are in Gamma(Γ) point. So they correspond to $k=0$. Instead the minima of conduction band are not at Γ point.

They correspond to a point different from Γ point.

Semiconductors that has this property are called indirect semiconductors.

→ In contrast GaAs has both Max. Valence band & Min. Conduction Band at Γ point.
So, it is called Direct semiconductor

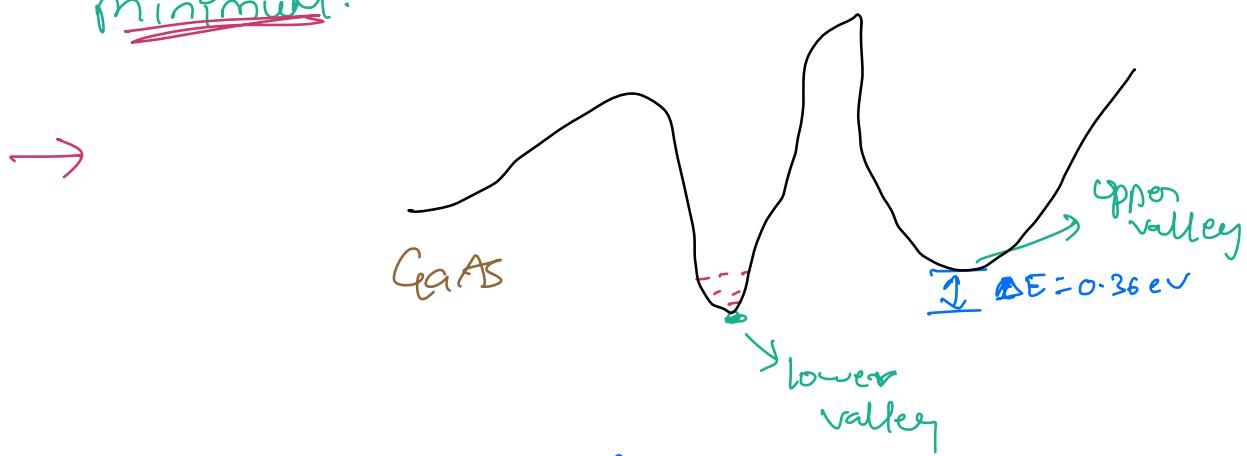
→ Direct semiconductors like GaAs have much much probability that the interaction of semiconductor with Electro magnetic Radiation" is able to induce a transition of electron from VB to CB

on Viceversa.

Low probability for Indirect
semiconductors

Eg:- Lasers made of Semiconductor is
made of GaAs than Ge or Si

→ GaAs has Absolute minimum at T point
and there is another minimum which is
close to Absolute minimum and this is
also important because when we consider
Equilibrium condition, majority of electrons
belong to states which are close to Absolute
minimum.

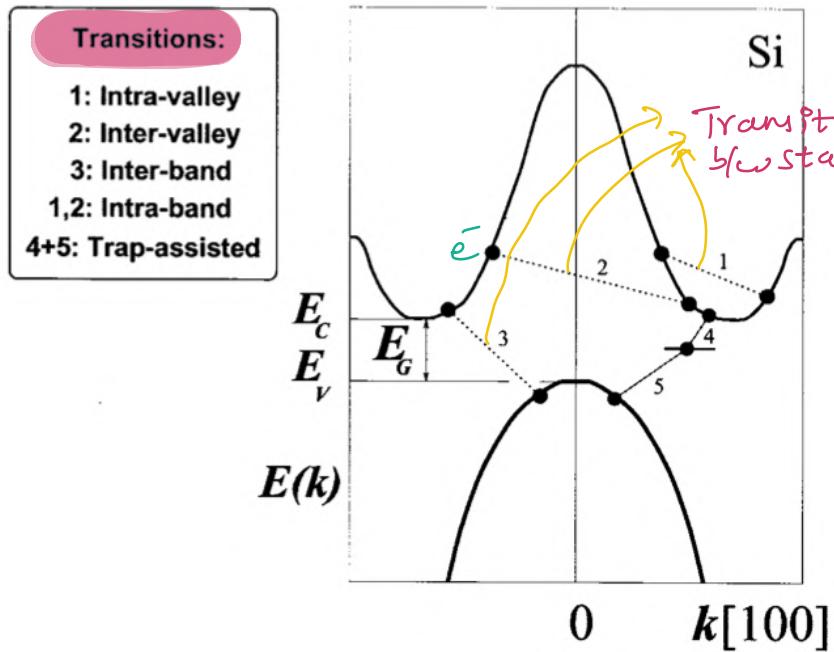


when an external force is applied electrons ..

move from lower valley to upper valley and if we observe the curvature of lower valley is smaller when compared to upper valley.

We will also study soon, that in a semiconductor that inertia of electrons to external forces is not related to "actual mass of the semiconductor" but is related to the "Curvature of the Band"

- So inertia of e^- in lower valley have low energy but are lighter. Consequently e^- in the upper valley have high energy but are heavier.
The consequence of this is that the material might become unstable
- There is a -ve slope in the $V_{(vs)} I$ graph and this might introduce oscillations and this is actually exploited to produce oscillations.



T. 21.15: Due rami delle bande del silicio nella direzione [100].

- If e^- is subjected to external perturbation (weak perturbation) it may move along the Branch. Indicating that due to external perturbation, the energy and momentum of electrons are changing.
- In crystals it may happen that electrons may be subjected to perturbation that are not considered weak. The typical example of strong perturbation is collision.

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$e^- \rightarrow e^-$ collision

$e^- \rightarrow$ Atom collision

$e^- \rightarrow$ Impurity collision

$e^- \rightarrow$ boundary collision.

because of this e^- may change e^- Energy
and momentum in short amount of time
and \therefore we must consider these Transition
from initial state to final state

→ These transitions may be classified

- 1) Considering another object with which e^- is colliding
- 2) Observing where the initial and final state are.



→ Intra Band transitions are very fast
other Transition are rather slow.

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సుమిత్ర పన్నల

→ Inter Band transitions

ca:- VB to CB
valence conduction
Band Band

This transition is called electron-hole generation transition.

Generation & Recombination phenomenon are caused to Inter Band Transition.

→ Trap-Assisted Transition is because of defects or imperfections in the crystal structure.

* Density of States *

For this we take a simple figure



VI. DENSITY OF STATES

Considering the quantum case in the parabolic-band approximation and one dimension, with m_a the effective mass, figure 5 provides a schematic view of the definition of density of states. The number of k states belonging to the $[k, k + \Delta k]$ interval is, by construction, equal to the number of energy states belonging to the $[E, E + \Delta E]$ interval. On the other hand, being the distribution of k states uniform, the number of states in the $[k, k + \Delta k]$ interval is $Q_k \Delta k$. If Δk is made smaller and smaller, one defines a function $g(E)$ such that

$$g(E) dE = Q_k dk. \quad (42)$$

Since the relation $E(k) = \frac{\hbar^2 k^2}{(2m_a)} + V_0$ is non linear, $g(E)$ is not a constant; in fact,

$$g(E) = Q_k \frac{dk}{dE} = \frac{Q_k}{dE/dk}. \quad (43)$$

On the other hand,

$$\frac{dE}{dk} = \frac{\hbar^2}{m_a} k, \quad k = \frac{1}{\hbar} \sqrt{2m_a(E - V_0)}, \quad (44)$$

namely, letting $E_e = E - V_0$,

$$\frac{dE_e}{dk} = \frac{\sqrt{2}\hbar}{\sqrt{m_a}} \sqrt{E_e}. \quad (45)$$

Replacing (45) in (43) yields

$$g(E_e) = \frac{Q_k \sqrt{m_a}}{\sqrt{2}\hbar} \frac{1}{\sqrt{E_e}}. \quad (46)$$

The dependence of g on the inverse square root of E_e is due to the fact that a one-dimensional case is considered. The dependence is different in the two- or three-dimensional cases. Considering for instance the two-dimensional case, assuming isotropy for simplicity, one has

$$E_e = \frac{\hbar^2}{2m_a} (k_1^2 + k_2^2), \quad k_1^2 + k_2^2 = \frac{2m_a}{\hbar^2} E_e, \quad (47)$$

which represents a circumference of radius $k = \sqrt{2m_a E_e}/\hbar$. If the radius is increased by dk , the area of the annular strip between the circumference of radius $k + dk$ and that of radius k is $\pi(k + dk)^2 - \pi k^2 \simeq \pi k dk$. Expressing k in terms of energy yields

$$k dk = \frac{\sqrt{2m_a E_e}}{\hbar} \frac{\sqrt{2m_a} dE_e}{\hbar 2 \sqrt{E_e}} = \frac{m_a}{\hbar^2} dE_e. \quad (48)$$

On the other hand, the number of states in the strip is

$$Q_k \pi k dk = Q_k \pi \frac{m_a}{\hbar^2} dE_e. \quad (49)$$

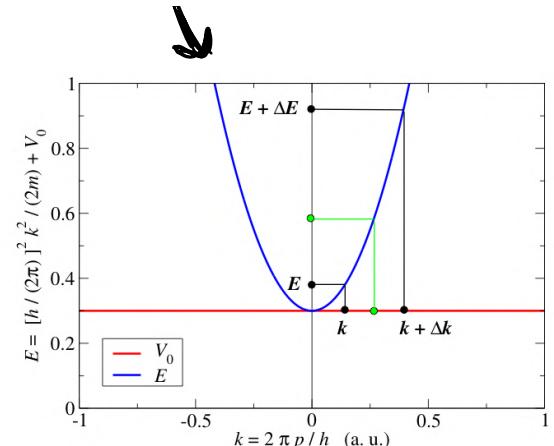


Fig. 5. Construction of the density of states $g(E)$ in the one-dimensional case.

It follows

$$g(E_e) = Q_k \pi \frac{m_a}{\hbar^2} = \text{const.} \quad (50)$$

In three dimensions,

$$E_e = \frac{\hbar^2}{2m_a} (k_1^2 + k_2^2 + k_3^2), \quad k_1^2 + k_2^2 + k_3^2 = \frac{2m_a}{\hbar^2} E_e, \quad (51)$$

which represents a spherical surface whose radius is, like before, $k = \sqrt{2m_a E_e}/\hbar$. If the radius is increased by dk , the volume of the shell between the sphere of radius $k + dk$ and that of radius k is $(4/3)\pi(k + dk)^3 - (4/3)\pi k^3 \simeq 4\pi k^2 dk$. Expressing k in terms of energy yields

$$k^2 dk = \frac{2m_a E_e}{\hbar^2} \frac{\sqrt{2m_a} dE_e}{\hbar 2 \sqrt{E_e}} = \sqrt{2} \frac{m_a^{3/2}}{\hbar^3} \sqrt{E_e} dE_e. \quad (52)$$

The number of states in the strip is

$$Q_k 4\pi k^2 dk = Q_k 4\pi \sqrt{2} \frac{m_a^{3/2}}{\hbar^3} \sqrt{E_e} dE_e, \quad (53)$$

whence

$$g(E_e) = Q_k \pi \frac{(2m_a)^{3/2}}{\hbar^3} \sqrt{E_e}. \quad (54)$$

The anisotropic case is treated in the same manner. Considering for instance the anisotropic form of (47),

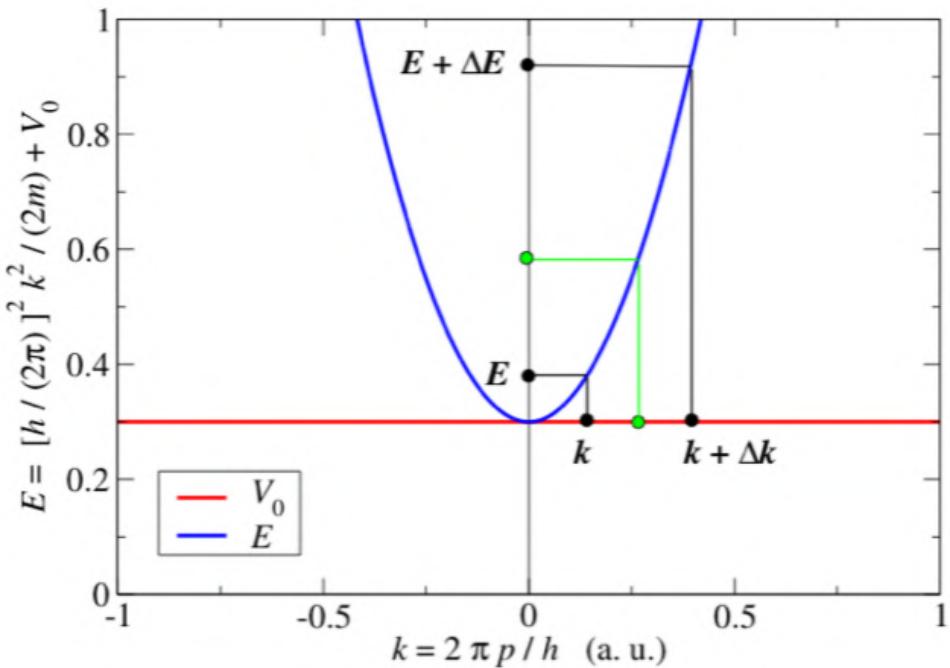
$$E_e = \frac{\hbar^2}{2} \left(\frac{k_1^2}{m_{a1}} + \frac{k_2^2}{m_{a2}} \right), \quad (55)$$

one defines $\eta_1 = k_1/\sqrt{m_{a1}}$ and $\eta_2 = k_2/\sqrt{m_{a2}}$, to find

$$\eta_1^2 + \eta_2^2 = \frac{2}{\hbar^2} E_e. \quad (56)$$

The rest of the procedure is identical to the one illustrated above.

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we assume the band is Parabolic and
we remember that $\langle k \rangle$ vector is discretized
and there is finite no. of $\langle k \rangle$ vectors in each
interval and they are equally spaced.

→ Consider a value of k and an other
value of $k + \Delta k$ possible values of k on
horizontal axis
Corresponding possible values of E along vertical axis.

$$k \rightarrow E$$

$$k + \Delta k \rightarrow E + \Delta E$$

• any value of ' k ' along the interval

$$'k' \rightarrow 'k + \Delta k'$$

→ values of ' k ' are equally spaced because ' k ' is discretized and has constant density.

The corresponding values of Energy are not equally spaced because the relationship b/w ' k ' & ' E ' is Non-linear. because it's Parabolic

→ we want to understand how Energy points are distributed wrt ' k '.

→ ' k ' are discrete but are very dense so, we can consider ' k ' to be continuous and use Derivatives

Density of states $g(E)$ can be defined as

$$\boxed{g(E) dE = \Omega_k dk}$$

→ we take Δk smaller and smaller in order to make it infinitesimal and we count the no. of ' k ' vectors in these intervals.

→ As ' k ' vectors are equally distributed the total no. of ' k ' vectors in the interval

$$k \text{ & } k + \Delta k$$

is equal to a constant density

$$Q(k) \Delta k \approx Q(k) dk$$

(for smaller values of Δk)

→ For each ' k ' there corresponds an energy. ∴ The no. of energy in vertical segment of the graph is equal to the value of ' k ' in the horizontal segment.

→ But the values of Energy are not Equally distributed so we must Introduce a function $g(E)$ depending on energy.

$$\therefore g(E) dE = \Omega_k dk \quad \text{---(1)}$$

$g(E)$: is a very important function it is called Density of States in Energy

Ω_k : Is the density of k vectors along the k axis

→ we also have another Relation when the relation b/w Energy and Momentum is parabolic.

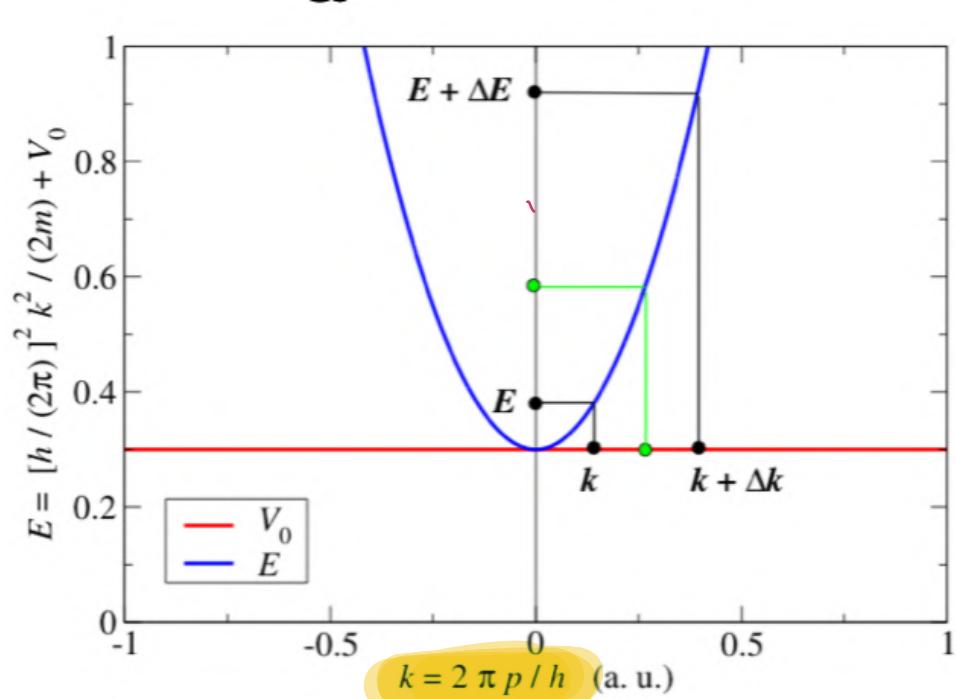
If we use ' P ' has momentum we would have

$$E = P \cdot E + \frac{P^2}{2}$$

αm

It can be demonstrated that $\langle \hat{p} \rangle$ can be related to average momentum and the fact of proportionality is the Planck's constant (\hbar) divided by 2π

We see this relation on the x -axis of the figure. $\langle \hat{p} \rangle = \frac{2\pi P}{\hbar}$



$$P = \frac{\hbar k}{2\pi} = \hbar \tilde{k}$$

\hbar : Reduced Planck's constant

$\therefore E = \text{Total Energy}$

$$E = \frac{p^2}{2ma} + P.E$$

$P.E = V_0$
potential Energy

$$E = \frac{\hbar^2 k^2}{2ma} + V_0$$

②

From ① & ②

$$g(E) = \frac{Q_K dK}{dE} \Rightarrow \frac{Q_K}{\left(\frac{dE}{dk} \right)}$$

③

$$\frac{dE}{dk} = \frac{d}{dk} \left[\frac{\hbar^2 k^2}{2ma} + V_0 \right]$$

$$\frac{dE}{dk} = \frac{\hbar^2 k}{ma}$$

$\therefore V_0 = \text{constant}$

$$\& \quad k = \frac{1}{\hbar} \sqrt{2ma(E - V_0)}$$

$$E - V_0 = E_e$$

Total Energy Potential energy Kinetic energy

$$\Rightarrow E_e = E - V_0$$

$$\boxed{\frac{dE_e}{dk} = \frac{\sqrt{2}\hbar}{\sqrt{m_a}} \sqrt{E_e}} \quad \textcircled{4}$$

put $\textcircled{4}$ in $\textcircled{3}$

$$\boxed{g(E_e) = \frac{Q_k \sqrt{m_a}}{\sqrt{2}\hbar} \frac{1}{\sqrt{E_e}}} \quad \downarrow$$

This applies when ' k ' is one dimensional

\rightarrow when we consider 2-dimensional case
 The density of states comes out to be different even though it is calculated same way.

$$E_e = \frac{\hbar^2}{2m_a} (k_1^2 + k_2^2), \quad k_1^2 + k_2^2 = \frac{2m_a}{\hbar^2} E_e, \quad (47)$$

Because, in 2D the k -E has the

above expressions because we have two components of ' k ' (k_1 & k_2)

$$\text{so the } k = \frac{\hbar^2}{2m} (k_1^2 + k_2^2)$$

→ The Geometrical construction also changes because in 1D we take

k and increase by little to

$(k + \Delta k)$ and correspondingly with the Energy corresponding to ' k '.

→ But, when we consider 2D and we look at

$$k_1^2 + k_2^2 = \frac{2m_a}{\hbar^2} E_e$$

This is a Circle

$$\text{whose Radius} = \sqrt{\frac{2m_a}{\hbar^2} E_e}$$

$$\nabla \quad v_l$$

$$E_e = \frac{\hbar^2}{2m_a} (k_1^2 + k_2^2), \quad k_1^2 + k_2^2 = \frac{2m_a}{\hbar^2} E_e, \quad (47)$$



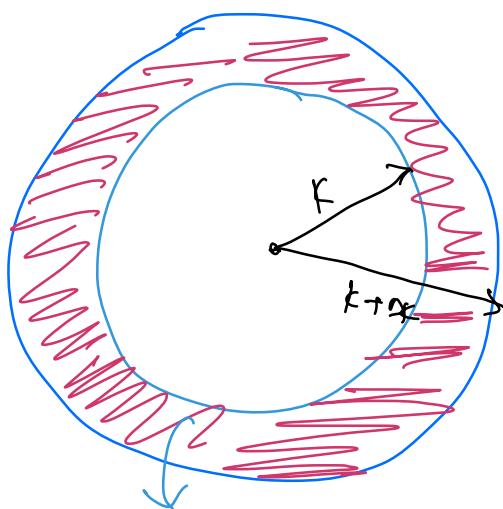
which represents a circumference of radius $k = \sqrt{2m_a E_e}/\hbar$. If the radius is increased by dk , the area of the annular strip between the circumference of radius $k + dk$ and that of radius k is $\pi(k + dk)^2 - \pi k^2 \simeq \pi k dk$. Expressing k in terms of energy yields

$$k dk = \frac{\sqrt{2m_a E_e}}{\hbar} \frac{\sqrt{2m_a} dE_e}{\hbar 2\sqrt{E_e}} = \frac{m_a}{\hbar^2} dE_e. \quad (48)$$

On the other hand, the number of states in the strip is

$$Q_k \pi k dk = Q_k \pi \frac{m_a}{\hbar^2} dE_e. \quad (49)$$

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$$\begin{aligned} dA &= \pi(k_f + dk)^2 - \pi k^2 \\ &= \pi k dk \end{aligned}$$

we know from above that



$$k dk = \frac{\sqrt{2m_a E_e}}{\hbar} \frac{\sqrt{2m_a} dE_e}{\hbar 2\sqrt{E_e}}$$

$$k dk \Rightarrow \frac{m_a}{\hbar^2} dE_e$$

$$E_e = \frac{P^2}{2m_a} \Rightarrow P = \hbar k$$

$$E_e \Rightarrow \frac{\hbar^2 k^2}{2m_a}$$

$$k = \frac{\sqrt{2m_a E_e}}{\hbar}$$

$$\frac{dE_e}{dk} = \frac{\sqrt{2} \hbar \sqrt{E_e}}{\sqrt{m_a}}$$

→ on the other hand, the no. of states in the strip is

$$\Omega_F \pi k dF = \Omega_F \pi \frac{m_q}{\hbar^2} dE_e$$

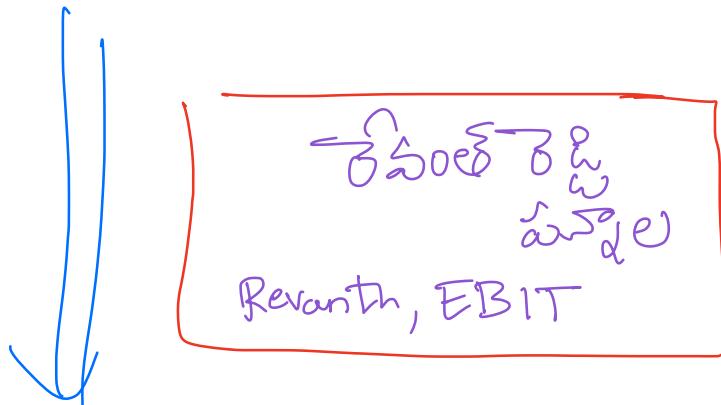
Density of States in 2D

$$g(E) = \Omega_F \pi \frac{m_q}{\hbar^2}$$

constant

Conclusion:- In 2D when the relation
b/w energy and momentum is
parabolic the density of states is
constant -

→ In 3D procedure is same
and it is given in the



In three dimensions,

$$E_e = \frac{\hbar^2}{2m_a} (k_1^2 + k_2^2 + k_3^2), \quad \text{Sphere} \quad k_1^2 + k_2^2 + k_3^2 = \frac{2m_a}{\hbar^2} E_e, \quad (51)$$

which represents a spherical surface whose radius is, like before, $k = \sqrt{2m_a E_e / \hbar}$. If the radius is increased by dk , the volume of the shell between the sphere of radius $k + dk$ and that of radius k is $(4/3)\pi(k + dk)^3 - (4/3)\pi k^3 \simeq 4\pi k^2 dk$. Expressing k in terms of energy yields

$$k^2 dk = \frac{2m_a E_e}{\hbar^2} \frac{\sqrt{2m_a} dE_e}{\hbar 2 \sqrt{E_e}} = \sqrt{2} \frac{m_a^{3/2}}{\hbar^3} \sqrt{E_e} dE_e. \quad (52)$$

The number of states in the strip is

$$Q_k 4\pi k^2 dk = Q_k 4\pi \sqrt{2} \frac{m_a^{3/2}}{\hbar^3} \sqrt{E_e} dE_e, \quad (53)$$

whence

$$g(E_e) = Q_k \pi \frac{(2m_a)^{3/2}}{\hbar^3} \sqrt{E_e}. \quad (54)$$

$$g(E_e) \propto \sqrt{E_e}$$

in 3 Dimensions

Density of states in 3D is proportional
to square root of Energy.

$\therefore k \& P$ are related
we can make some deductions.

Density of States in the \mathbf{k} and \mathbf{r}, \mathbf{k} Spaces.

It is found

$$E_r(\mathbf{k} + \mathbf{g}) = E_r(\mathbf{k}), \quad E_r(-\mathbf{k}) = E_r(\mathbf{k})$$

↑ Scaled reciprocal lattice
This explains periodicity in lattice
Energy is even w.r.t momentum

where r is the index of the branch (band) and \mathbf{g} is a translational vector in \mathbf{k} space. The density of the \mathbf{k} vectors in the Brillouin zone is

$$\frac{N_c}{\tau_g} = \frac{\Omega/\tau_l}{\tau_g} = \frac{\Omega}{(2\pi)^3}.$$

Due to spin, the density of states in \mathbf{k} is

$$Q_k = 2 \frac{N_c}{\tau_g} = \frac{\Omega}{4\pi^3}.$$

Since the crystal is uniform, the density of states in \mathbf{r}, \mathbf{k} is

$$Q = \frac{Q_k}{\Omega} = \frac{1}{4\pi^3}.$$

(

$\textcircled{1}$

The density of ' f ' vectors in the Brillouin zone ?

i.e Q_f

$\textcircled{2}$

The total of ' f ' vectors in the Brillouin zone is equal to the total

no. of cells of the Direct lattice .

Density
of
 \mathbf{k} ' vectors

$$\frac{N_c}{T_g} = \frac{\text{Total no. of cells}}{\text{volume of the Brillouin zone}} = \frac{\Omega}{(2\pi)^3}$$

$$\frac{N_c}{T_g} = \frac{\Omega/T_L}{T_g} = \frac{\Omega}{(2\pi)^3}$$

→ Because of the Quantum property
spin .

Due to spin, the density of states in \mathbf{k} is

$$Q_k = 2 \frac{N_c}{T_g} = \frac{\Omega}{4\pi^3}.$$

Since the crystal is uniform, the density of states in \mathbf{r}, \mathbf{k} is

$$Q = \frac{Q_k}{\Omega} = \frac{1}{4\pi^3}.$$

→ Due to spin when an electron has

an Energy actually there correspond two possible Quantum states to that energy and they differ by Spin.

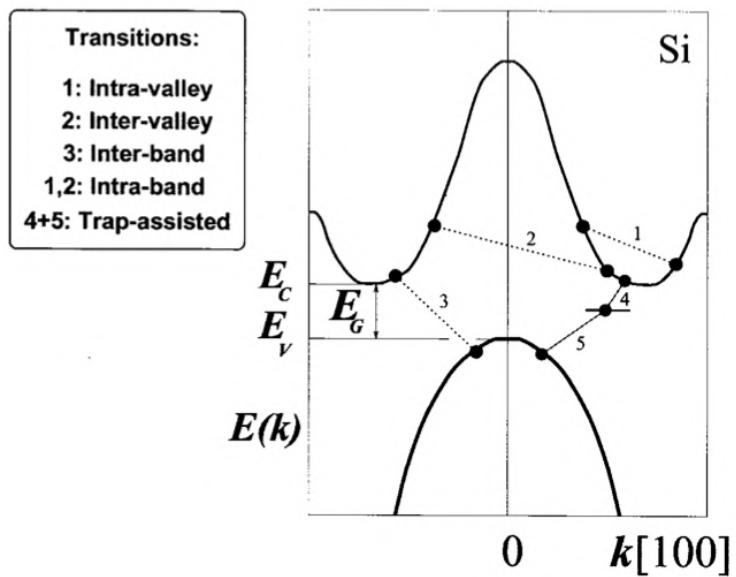
(x, k) Space is 6 Dimensional

$$\Omega = \frac{Q_k}{2} = \frac{1}{4\pi^3}$$

density in physical space when considering Uniform crystal.

* we must introduce a simplification in the description of the Bands because in the figure below there is a complicated shape of the Band

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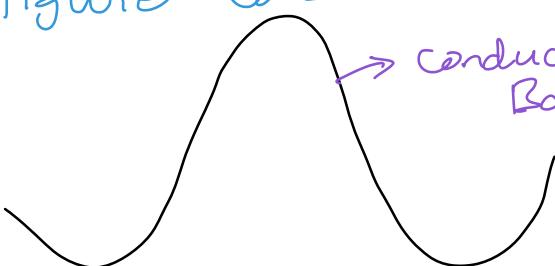
T. 21.15: Due rami delle bande del silicio nella direzione [100].

* In the above figure Conduction Band is described as . . .

The shape is inconvenient to describe the physical properties of the electrons that belong to the conduction Band.

In principle we should take full shape of the Band into consideration to describe properties of electrons.

Q: Do we actually need to consider the



whole Band !

Any No

Because, we remember from the other figures discussed above that the electrons of the conduction band belong to the state that are near the **Minima**.

So, if the e^-s sit near the Minima and we consider each minimum at a time then the form of Band that really matters is the form of the Band that is near the Minimum.

If we take a function and we consider a small portion of the function near the minimum you may think of the function by simplifying it by taking

Taylor expansion of the function.

Q So, what happens when we take Taylor expansion at the Minimum?

A The constant i.e at the minimum i.e E_c is taken as Other

1st, 2nd, ... order terms are taken

→ As, we are considering the Minimum

point the 1st derivative is zero

and then the next term is Quadratic

term and we stop the expansion.

→ By doing so, we get a Quadratic term in the Taylor expansion and we restore the PARABOLIC FORM, we

studied earlier.

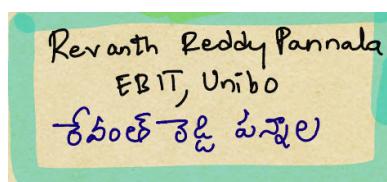
i.e parabolic form of Relation b/w Energy & Momentum ($P \propto K$) that applies in Free Space.

→ After, the complicity of introducing a Band, we eliminate it by by considering Parabolic approximation near the Minima.

→ Infact, this is called Parabolic band approximation.

We do the same for Valence Band.

We do Taylor expansion at the Maxima of the Valence Band.



Density of States in Energy — I

The number of values of \mathbf{k} within the Brillouin zone is so large that \mathbf{k} can be treated as a continuous variable. Let \mathbf{k}_a be the value of \mathbf{k} at the a th minimum of $E_r(\mathbf{k})$ within the Brillouin zone, for a fixed branch index r , and let $E_a = E_r(\mathbf{k}_a)$. At \mathbf{k}_a the Hessian matrix of $E_r(\mathbf{k})$ is symmetrical and positive definite, hence it can be diagonalized with positive real eigenvalues; as a consequence, the expansion of $E_r(\mathbf{k})$ around \mathbf{k}_a can be written as

$$E_r(\mathbf{k}) \simeq E_a + \frac{1}{2} \sum_{i=1}^3 \left(\frac{\partial^2 E_r}{\partial k_i^2} \right)_a (k_i - k_{ia})^2 \geq E_a, \quad a = 1, 2, \dots$$

Letting $E_{ea}(\mathbf{k}) \doteq E_r(\mathbf{k}) - E_a \geq 0$ and defining the inverse mass tensor at \mathbf{k}_a as the diagonal tensor of components

$$\frac{1}{m_{ia}} \doteq \frac{1}{\hbar^2} \left(\frac{\partial^2 E_r}{\partial k_i^2} \right)_a > 0$$

yields

$$E_{ea} = \sum_{i=1}^3 \frac{\hbar^2}{2m_{ia}} (k_i - k_{ia})^2$$

Taylor Expansion at the Minimum of the Conduction Band where

E_a = Minimum value of Conduction

The name of the ' \mathbf{k} ' at the Minimum is

' \mathbf{k}_a ' apart from GaAs the minimum is not the T point.
(Gamma)

K

D ... An min. the

→

Parabolic Approximation

$$E_r(\mathbf{k}) \simeq E_a + \frac{1}{2} \sum_{i=1}^3 \left(\frac{\partial^2 E_r}{\partial k_i^2} \right)_a (k_i - k_{ia})^2 \geq E_a, \quad a = 1, 2, \dots$$

Letting $E_{ea}(\mathbf{k}) \doteq E_r(\mathbf{k}) - E_a \geq 0$ and defining the inverse mass tensor at \mathbf{k}_a as the diagonal tensor of components

For Gaffs k_{ia} is at the T point i.e zero of ' \mathbf{k} '.

' \mathbf{k} ' has 3 components because it's a Vector.

k_i , here i is the index of the Components k_1, k_2, k_3

→ So, in parabolic Approximation we don't have 1st order terms and we consider only 2nd order terms for Approximation.

$$\rightarrow E_r(\mathbf{k}) = \boxed{E_a} + \frac{1}{2} \sum_{i=1}^3 \left(\frac{\partial^2 E_r}{\partial k_i^2} \right)_{k_i=k_{ia}} [k_i - k_{ia}]^2 \geq E_a$$

minimum of component "i" calculated at 'a'
 The Conduction band γ : Energy band

→ Since, $E_\gamma(k) \geq E_a$

kinetic energy

$$\therefore E_{ea}(k) = E_\gamma(k) - E_a \geq 0$$

a is the count or of Minimum
 c we encountered in the Density of states concept - $k(E)$

* → In the equation of Taylor expansion at the minima of CB -

$$\left(\frac{\partial^2 E_\gamma}{\partial k_i^2} \right)$$

The individual components of the derivative are not necessarily equal.

So, the curvature in all directions is

not necessarily same.

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→ we know that

$$\frac{\partial E_e}{\partial K} = \frac{\sqrt{2} \hbar \sqrt{\bar{E}_e}}{\sqrt{m_a}}$$

Letting $E_{ea}(K) \doteq E_r(K) - \bar{E}_a \geq 0$ and defining the inverse mass tensor at \mathbf{k}_a as the diagonal tensor of components

$$\frac{1}{m_{ia}} \doteq \frac{1}{\hbar^2} \left(\frac{\partial^2 E_r}{\partial k_i^2} \right)_a > 0$$

yields

$$E_{ea} = \sum_{i=1}^3 \frac{\hbar^2}{2m_{ia}} (k_i - k_{ia})^2$$



$$\bar{E}_{ea}(K) = E_r(K) - \bar{E}_a$$

$$\bar{E}_{ea} = \frac{\hbar^2 K^2}{2m_a}$$

Basic equation
 $T \cdot E = K \cdot \bar{E} + P \bar{E}$

$$\Rightarrow \frac{\partial \bar{E}_{ea}}{\partial K_a} = \frac{2 \hbar^2 K}{2m_a}$$

$$\Rightarrow \frac{\partial \bar{E}_{ea}}{\partial K_a} = \frac{\hbar^2 K}{m_a}$$

$$\Rightarrow \boxed{\frac{\frac{J^2}{2} E_{ea}}{2 k_i^2} = \frac{k_i^2}{m_a}}$$

$$\Rightarrow \frac{1}{m_{ia}} = \left(\frac{\frac{J^2}{2} E_{ea}}{2 k_i^2} \right) \cdot \frac{1}{r_i^2}$$

* * * :

$$E_{ea} = \sum_{i=1}^3 \frac{r_i^2}{m_{ia}} (k_i - k_{ia})^2$$

Index 'a' reminds that we are calculating from minimum 'a' at

(a) goes from 1 to 6

$\rightarrow m_{ia} \rightarrow$ ^{ith} component of effective Mass

$$E_{\text{ca}} = \sum_{i=1}^3 \frac{k^2}{2m_i a} (k_i - k_{ia})^2$$

The energy in the Conduction Band
is the quadratic form.

We should be happy because we have
recovered a Quadratic Relation b/w
Energy and Free particle.

→ This is not exactly equal to the
Relation we derived for a Free particle
Because, The minimum is displaced
w.r.t origin $(k_i - k_{ia})^2$

The 2nd difficulty is, in many
cases the effective Mass ($m_i a$)
is different in different directions

K_1, K_2, K_3

$\left(\begin{array}{c} \downarrow \\ m_{ia} \end{array} \right) \rightarrow \therefore$ It is called
Inverse Effective
mass Tensor.

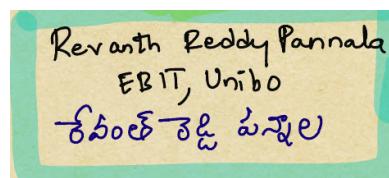
$\rightarrow \textcircled{Q}$ Why is this mass $\left(\begin{array}{c} \downarrow \\ m_{ia} \end{array} \right)$ important?

It can be demonstrated that the
Inertia of the **electron** when e^- is
subjected to perturbation is given by

m_{ia} not by the mass of free e^-



The density of states is similar to the
calculation we have done above.



Density of States in Energy — II

Letting $\eta_i = (\hbar/\sqrt{2m_{ia}})(k_i - k_{ia})$, the above can be recast as

$$E_{ea} = \sum_{i=1}^3 \eta_i^2 = \eta^2, \quad \eta > 0$$

From the definition of η_i it follows

$$dk_i = \frac{\sqrt{2m_{ia}}}{\hbar} d\eta_i, \quad d^3k = dk_1 dk_2 dk_3 = 2\frac{\sqrt{2}}{\hbar^3} m_{ea}^{3/2} d^3\eta$$

with $m_{ea} \doteq (m_{1a}m_{2a}m_{3a})^{1/3}$. Turning to polar coordinates

$$\eta_1 = \eta \sin \theta \cos \phi, \quad \eta_2 = \eta \sin \theta \sin \phi, \quad \eta_3 = \eta \cos \theta$$

yields $d^3\eta = \eta^2 d\eta \sin \theta d\theta d\phi$. The term $\eta^2 d\eta$ is found from

$$2\eta d\eta = dE_{ea}, \quad d\eta = \frac{dE_{ea}}{2\sqrt{E_{ea}}} \Rightarrow \eta^2 d\eta = \frac{1}{2} \sqrt{E_{ea}} dE_{ea}$$

In conclusion, remembering that $Q_k = \Omega/(4\pi^3)$, one finds for the number of states in d^3k and in the vicinity of the a th minimum of $E_r(\mathbf{k})$:

$$dN_a = Q_k d^3k = \frac{\Omega}{4\pi^3} 2\frac{\sqrt{2}}{\hbar^3} m_{ea}^{3/2} \frac{1}{2} \sqrt{E_{ea}} dE_{ea} \sin \theta d\theta d\phi$$

The number of states in the strip is

$$Q_k 4\pi k^2 dk = Q_k 4\pi \sqrt{2} \frac{m_a^{3/2}}{\hbar^3} \sqrt{E_e} dE_e, \quad (53)$$



Similar only
difference is
 m_{ea}

Density of States in Energy — III

Integration over the angles yields 4π , whence

$$\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} dN_a = \Omega \frac{\sqrt{2}}{\pi^2 \hbar^3} m_{ea}^{3/2} \sqrt{E_{ea}} dE_{ea} \doteq g_a(E_{ea}) dE_{ea}$$

where $g_a(E_{ea})$ is the density of states in energy around the a th minimum. If there are M_C absolute minima it follows $E_1 = \dots = E_{M_C} \doteq E_C$, whence $E_{ea} \leftarrow E_r - E_C \doteq E_e$. Summing g_a over the absolute minima yields

$$g(E_e) \doteq \sum_{a=1}^{M_C} g_a = \Omega \frac{\sqrt{2}}{\pi^2 \hbar^3} M_C m_e^{3/2} \sqrt{E_e}$$

where the average effective mass of the electrons is defined as

$$M_C = 6 \text{ in silicon}$$

$$M_C = 1 \text{ in GaAs} \quad m_e \doteq \left(\frac{1}{M_C} \sum_{a=1}^{M_C} m_{ea}^{3/2} \right)^{2/3}$$

The density of states in energy and \mathbf{r} is given by

$$M_C = 4 \text{ in Ge} \quad \gamma \doteq \frac{g}{\Omega} = \frac{\sqrt{2}}{\pi^2 \hbar^3} M_C m_e^{3/2} \sqrt{E_e}$$

This equation is the density of states at a particular \mathbf{r}
For a Brillouin zone $1 \leq a \leq 6$

M_C : Total no. of the Conduction Minima
of the Absolute minima of the conduction
Band.

Density of States in Energy — IV

In the case of holes it is necessary to consider the maxima of E_r . Let \mathbf{k}_a be the value of \mathbf{k} at the a th maximum of $E_r(\mathbf{k})$; there, the Hessian matrix of $E_r(\mathbf{k})$ is symmetrical and negative definite, hence it can be diagonalized with negative real eigenvalues:

$$E_r(\mathbf{k}) \simeq E_a + \frac{1}{2} \sum_{i=1}^3 \left(\frac{\partial^2 E_r}{\partial k_i^2} \right)_a (k_i - k_{ia})^2 \leq E_a, \quad a = 1, 2, \dots$$

Letting $E_{ha}(\mathbf{k}) \doteq E_a - E_r(\mathbf{k}) \geq 0$ and defining

$$\boxed{\frac{1}{m_{ia}} \doteq -\frac{1}{\hbar^2} \left(\frac{\partial^2 E_r}{\partial k_i^2} \right)_a > 0}$$

yields $E_{ha} = \sum_{i=1}^3 \frac{\hbar^2}{2m_{ia}} (k_i - k_{ia})^2$

*ve is chosen
to avoid ve
sign of 2nd
derivative*

The same calculation as for the minima provides

$$g(E_h) \doteq \sum_{a=1}^{M_V} g_a = \Omega \frac{\sqrt{2}}{\pi^2 \hbar^3} M_V m_h^{3/2} \sqrt{E_h}$$

where $E_{ha} \leftarrow E_h \doteq E_V - E_r$, M_V is the number of absolute maxima, and m_h is the average effective mass of the holes.

Now, we must repeat the analysis for the valence band. We remember that in valence band in semiconductors of interest we have only two branches

and these two branches are centered in the origin.

Second derivatives at Maximum

-ve

$$\therefore \text{we choose } \frac{1}{m_a} = -\frac{1}{t^2} \frac{\partial^2 E_k}{\partial k^2}$$

$M_V = 2$

for Si, Ge & GaAs
semiconductors of
Interest.

* From now on we are going to use
Parabolic Band Approximation
in our Analysis.

Good bye and

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Examples: Band Structures of Si, Ge, GaAs — I

The crystals of Silicon, Germanium, and Gallium Arsenide are of the cubic, face-centered type. The reciprocal lattices have the cubic, body-centered structure. The lattice constants at $T = 300$ are

$$a(\text{Si}) = 5.43 \text{ \AA}, \quad a(\text{Ge}) = 5.66 \text{ \AA}, \quad a(\text{GaAs}) = 5.65 \text{ \AA}.$$

In these three semiconductors, the valence band is made of two branches of $E(\mathbf{k})$, spherically symmetric around $\mathbf{k} = 0$. The two branches have the same absolute maximum E_V at $\mathbf{k} = 0$, but different curvatures.

The curvature of E along the direction of k_i is $c = E''/(1+E'^2)^{3/2}$, where the primes indicate the derivatives with respect to k_i . The curvature radius is $\rho = 1/c$.

At the maximum it is $E' = 0$, whence the masses $m \sim 1/E''$ are proportional to ρ .

The holes belonging to the branch of larger mass are called “heavy”, those belonging to the other branch are called “light”.

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Examples: Band Structures of Si, Ge, GaAs — II

In the valence band and in the parabolic-band approximation, the surfaces at constant energy have the form

$$E_{hr} = E_V - E_r(\mathbf{k}) = \sum_{i=1}^3 \frac{\hbar^2}{2m_{hr}} k_i^2,$$

$$\frac{1}{m_{hr}} = -\frac{1}{\hbar^2} \left(\frac{\partial^2 E_r}{\partial k_i^2} \right)_{k=0} > 0 \quad (\text{independent of } i),$$

where $r = h$ for the heavy holes and $r = l$ for the light ones. The surfaces $E_{hh} = \text{const}$ and $E_{hl} = \text{const}$ are spheres.

	$m_{hl}(T_a)/m_0$	$m_{hh}(T_a)/m_0$
Ge	0.04	0.3
Si	0.16	0.5
GaAs	0.12	0.5

In valence band for each of the two branches of the valence band comes out that effective masses

$$\begin{pmatrix} 1 \\ m_{hr} \end{pmatrix} = \begin{pmatrix} 1 \\ m_{hr} \end{pmatrix}_{r=\text{lighter hole}} \quad r=\text{Heavy}$$

holes

i.e. The branches are isotropic
their properties are same in all directions
of ' k ' space.

$$\frac{\partial^2 E_r}{\partial k_1^2} = \frac{\partial^2 E_r}{\partial k_2^2} = \frac{\partial^2 E_r}{\partial k_3^2}$$

When we want to describe or indicate
the values of these masses. Instead of
indicating absolute values of the masses
it is more convenient to express the ratio
by $\frac{\text{mass of particle}}{\text{mass of free } e^-}$

	Hole, light Branch	Hole, heavy Branch
	$m_{hl}(T_a)/m_0$	$m_{hh}(T_a)/m_0$
Ge	0.04	0.3
Si	0.16	0.5
GaAs	0.12	0.5

The effective mass depends on
Temperature.

It is the same way as Lattice constant
depends on Temperature of Lattice. As
 $T_{lattice} \uparrow$ Lattice will

Temp ↑ \rightarrow Expand.)
i.e The lattice constant will expand
The characteristic vectors of the
Direct lattice will expand.

The characteristic vectors b_1, b_2, b_3
of Reciprocal lattice will contract.

and the $E(k)$ relation will deform
which is defined in the First Brillouin
Zone. curvature will change and

the curvature $\frac{\partial^2 E_r}{\partial k_i^2}$ is the

Inverse of the Mass m_α

However, This dependence is very
very small and in majority of these
cases it can be neglected.

Examples: Band Structures of Si, Ge, GaAs — III

The conduction band of Si, Ge, and GaAs has only one branch. However, the absolute minimima are placed differently.

- ▷ In GaAs there is only one absolute minimum at $\mathbf{k} = 0$, with spherical symmetry. In the parabolic-band approximation, the surfaces at constant energy have the form

$$E_{ea} = E(\mathbf{k}) - E_C = \sum_{i=1}^3 \frac{\hbar^2}{2m_{ea}} k_i^2, \quad a = 1,$$

$$\frac{1}{m_{ea}} = \frac{1}{\hbar^2} \left(\frac{\partial^2 E}{\partial k_i^2} \right)_{k=0} > 0 \quad (\text{independent of } i).$$

- ▷ In Si, there are six absolute minima, grouped into three pairs. The pairs are placed along the [100], [010], and [001] directions, respectively, and are symmetrical around $\mathbf{k} = 0$:

$$[100] : (\pm k_m, 0, 0), [010] : (0, \pm k_m, 0), [001] : (0, 0, \pm k_m),$$

where $k_m = 0.85 k_B > 0$, with k_B the extension of the first Brillouin zone.

For Germanium there are Four Minimas

$k_B =$ Distance b/w Gamma point and
X' point.

So it is the extension of Brillouin zone
on one side of the origin.

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Examples: Band Structures of Si, Ge, GaAs — IV

In the conduction band of Si, and in the parabolic-band approximation, the surfaces at constant energy are ellipsoids of revolution about the [100], [010], or [001] axes:

$$[100]: E_{e1} = E(\mathbf{k}) - E_C = \frac{\hbar^2}{2} \left[\frac{(k_1 - k_m)^2}{m_L} + \frac{k_2^2}{m_t} + \frac{k_3^2}{m_t} \right],$$

K-E

$$[010]: E_{e2} = E(\mathbf{k}) - E_C = \frac{\hbar^2}{2} \left[\frac{k_1^2}{m_t} + \frac{(k_2 - k_m)^2}{m_L} + \frac{k_3^2}{m_t} \right],$$

$$[001]: E_{e3} = E(\mathbf{k}) - E_C = \frac{\hbar^2}{2} \left[\frac{k_1^2}{m_t} + \frac{k_2^2}{m_t} + \frac{(k_3 - k_m)^2}{m_L} \right].$$

Similarly, E_{e4} , E_{e5} , E_{e6} are derived from E_{e1} , E_{e2} , E_{e3} , respectively, by letting $k_m \leftarrow -k_m$. The masses m_L and m_t are called *longitudinal* and *transverse mass*, respectively.

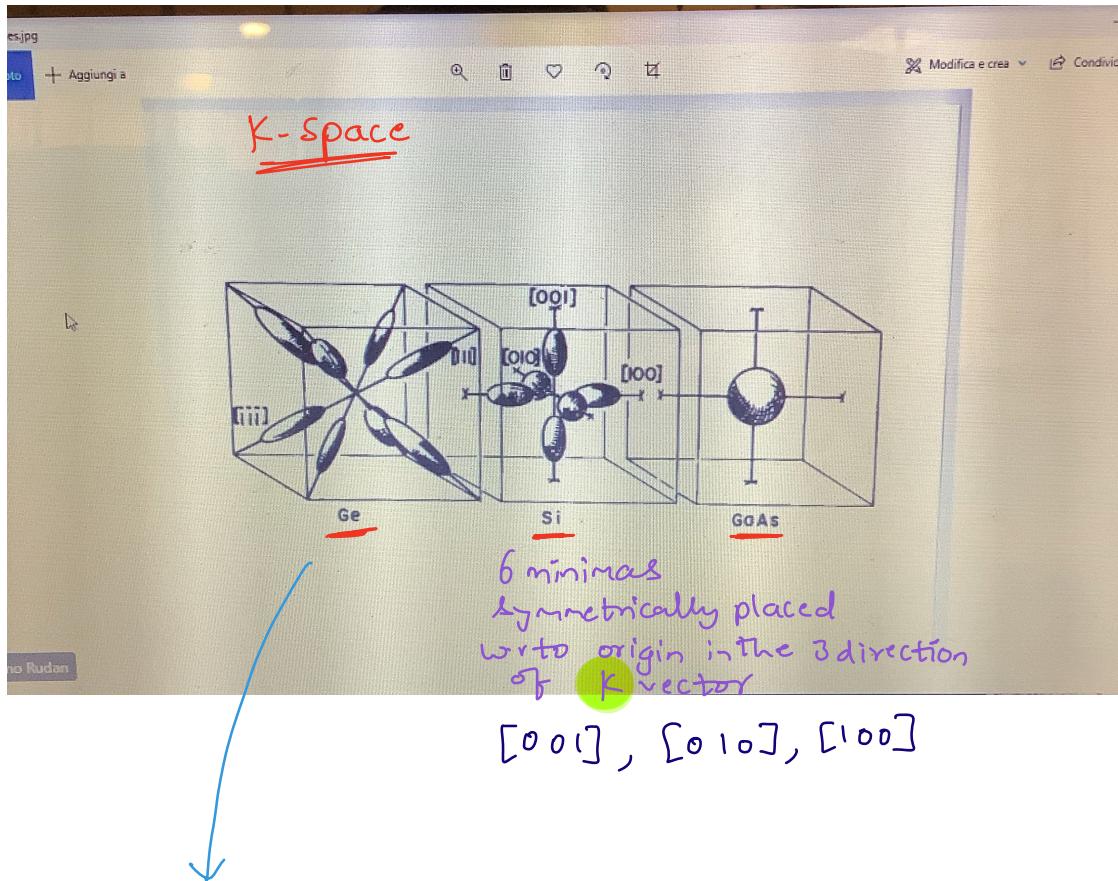
- ▷ In the conduction band of Ge, and in the parabolic-band approximation, there are eight ellipsoids of revolution about [111]-type axes, and the boundary of the first Brillouin zone is in the center of the ellipsoids ($k_m = k_B$). Thus, only four absolute minima must be accounted for.

* * For GaAs

$$E_{ha} = \sum_{i=1}^3 \frac{\hbar^2}{2m_{ia}} (k_i - k_{ia})^2$$

Ans

because it has only absolute
minima about the Gamma point.



8 minima and they are
placed along $\langle 111 \rangle$ directions $\langle \bar{1}\bar{1}\bar{1} \rangle$

Examples: Band Structures of Si, Ge, GaAs — V

In the conduction band the values of the masses are:

	^{mass} longitudinal	^{transversal} mass
	$m_l(T_a)/m_0$	$m_t(T_a)/m_0$
Ge	1.6	0.082
Si	0.97	0.19
GaAs		0.068

^{mass}
GaAs has
 → least
Mass

It is worth noting that:

- The electron mass in GaAs is much smaller than in Si or Ge, which explains the much higher electron mobility of GaAs. This does not hold for holes. *GaAs is a Compound Semiconductor*
- The secondary minimum of GaAs at $E_C + \Delta E$, with $\Delta E \simeq 0.36$ eV, has a larger mass. Electrons making a transition to the upper valley become “heavier”. This gives rise to a negative differential resistivity in the material (i.e., to an operating region where the current density decreases as the electric field increases).
- GaAs has a *direct gap*, as the minimum of the conduction band and the maxima of the valence band occur at the same \mathbf{k} . Instead, Si and Ge have an *indirect gap*. In direct-gap semiconductors the probability of optical generation-recombination events is much higher, which explains why lasers are typically made of GaAs.

→ In the figure above Mass of GaAs is smaller than Si, Ge.

We know that Mass as inertia of a particle when we apply an external

Electric Field if the Mass of the particle is smaller we expect they react faster (The switching is faster).

We expect GaAs has better performance in terms of current & velocity than Si, Ge.

This is True.

→ On the other hand, there is a difficulty because it is a compound semiconductor and it is difficult to manufacture GaAs technology.

→ So, The enhancement in speed and performance can be obtained for instance with silicon simply by scaling i.e by making the device smaller and this is much much easier than GaAs.

→ For Ge, Si

Longitudinal Mass

>>

Transversal mass

That means that we have mixture of Heavy and light electrons & the properties are averaged.

→ It would be preferable in Si to have only light electrons; this can be possible. If it is subjected to mechanical tension the positions of the valleys change and we may manage to displace the valleys that only Transversal valleys are populated & longitudinal valleys are not populated..

