

## Lecture-4

"ఇ తో రో గణకతాను నుంచి!"

### Elettroni e lacune nei semiconduttori

Now, we start an other Topic.

→ When we want to consider the Transport properties of semiconductor we must consider a no. of Particles.

electrons  $\leftrightarrow$  holes  $\leftrightarrow$  both

→ This makes practically impossible to consider individually dynamics of each particle.

This is impossible in principle because Quantum Mechanics prevents us from doing that.

If we wanted to use classical Mechanics it would be practically impossible to consider independently the motion of each particle because of the enormous

No. of Particles.

- The only way to proceed is using some statistics.

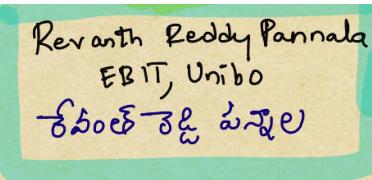
When we use statistics we denounce certain information and are content with information that we can acquire by taking the Average.

- In order to start using statistics we introduce a function that we call "  
"Distribution function"

Distribution function for now is a function that depends on one index and depends also on Time.

$$f_S(t)$$

time  
Index



### Discrete Distribution Function

$$f_1, f_2, \dots, f_s, \dots \quad f_s = f_s(t)$$

is the number of objects at time  $t$  in the  $s$ th subdomain. It is

$$f_s = C_s \Phi_s,$$

where  $C_s$  is the number of states in the  $s$ th subdomain and  $\Phi_s \geq 0$  is the fraction of occupied states.  $\Phi_s$  is also the occupation probability of a state if Pauli's principle holds  $\Rightarrow \Phi_s \leq 1$ . It is

$$C_s = Q_s \omega_s,$$

where  $Q_s$  is the density of states and  $\omega_s$  is the volume of the  $s$ th subdomain. The total number of objects is

$$\sum_s f_s = \sum_s C_s \Phi_s = \sum_s Q_s \omega_s \Phi_s.$$

Q What is the meaning of Distribution Function ?

The distribution function tries to describe objects that are in some Physical

Domain .

ex:- (i) Particles in Space

(ii) Particles in Reciprocal Space

(iii) Particles in the Combination of  
Direct & Reciprocal Space

→ we know that we can not acquire  
Individual Information about dynamics  
of each particle.

→ So, what we do is to divide the  
domain into subdomains and then  
we can be interested in -

Q How many particles are in  
the subdomain 1, 2..?  
at time  $t$ ?

ex:- Students & faculty

How many are in class A, B, C, D

at a particular instant of  
Time

not knowing individually which student is present in each class

This no. is called

$$f_S = f_S(t)$$

calculated at time  $t$

→ If class <sup>room</sup>A has 100 seats and no. of seats occupied by student is 20%. we can calculate the no. of students in class A

$$= \text{no. of seats} \times \frac{\text{fraction of seats occupied}}{\text{students}}$$



language of physics

→ If  $C_S$  the no. of states in the  $S^{th}$  subdomain

&  $\phi_S$  fraction of occupied states

Then the product will be no. of particles that are in the sub domain.

→ whenever we are considering electrons  
 we must consider a principle called  
 Pauli Principle such that a  
 state can be occupied atmost  
 by one electron. 0  $\leftrightarrow$  1

"Pauli's exclusion principle"

Translated each seat can be occupied  
 by only one student.

$$\phi_s \leq 1 \quad \begin{array}{l} \text{(probability)} \\ \text{of electron} \\ \text{occupying a} \\ \text{state} \end{array}$$

→  $C_s$  The no. of states in  $s^{\text{th}}$  domain

$$C_s = \alpha_s w_s$$

$\downarrow$  density of \_\_\_\_\_

$\downarrow$  volume of the  $s^{\text{th}}$  state

states

$\therefore$  Total no. of objects is

$$\sum_s f_s = \sum_s C_s \phi_s = \sum_s \Omega_s w_s \phi_s$$

For the moment we have been using  
a discrete index -

→ In Real life we will use continuous  
vectors.

### Continuous Distribution Function

Let  $\omega_s \approx d\omega$ ,  $C_s \approx dC = Q d\omega$  with  $Q = Q(\omega, t)$ . Similarly,  
 $\Phi_s \rightarrow \Phi(\omega, t)$ ,  $f_s \rightarrow f(\omega, t)$ . If  $d\omega = d^3r d^3k$ :

$$f = f(\mathbf{r}, \mathbf{k}, t), \quad \Phi = \Phi(\mathbf{r}, \mathbf{k}, t).$$

The total number of objects is

$$\iint f d^3r d^3k = \iint Q \Phi d^3r d^3k.$$

The number of objects in  $d^3r$  (concentration) is

$$\int f d^3k = \int Q \Phi d^3k.$$

Here it is  $Q = \text{const}$ . In crystals, the integrals are extended over  
the first Brillouin zone  $B$ . Let

$$\begin{cases} E = E(k_1, k_2, k_3) \\ \alpha = \alpha(k_1, k_2, k_3) \\ \beta = \beta(k_1, k_2, k_3) \end{cases} \quad \begin{cases} k_1 = k_1(E, \alpha, \beta) \\ k_2 = k_2(E, \alpha, \beta) \\ k_3 = k_3(E, \alpha, \beta) \end{cases}$$

$$H(E, \alpha, \beta) = \left[ \frac{\partial(k_1, k_2, k_3)}{\partial(E, \alpha, \beta)} \right]$$

∴ in continuous case volume of each subdomain becomes infinitesimal.

$$w_s \approx dw \quad C_s \approx dc = Q dw$$

volume                      with       $Q = Q(w, t)$

$$\phi_s = \underbrace{\phi(w, t)}_{\text{continuous function in } w \text{ & } t} \quad f_s \geq \underbrace{f_s(w, t)}_{}$$

→ Q what is ' $w$ '?

In our case we consider a space that is made of Union of physical space whose coordinates are  $\gamma_1, \gamma_2, \gamma_3$  & the

$\gamma$ -Space

$\gamma$ -vector has units inverse of Length.

$\gamma \rightarrow$  unit of length.

→ The distribution function becomes

a function of position of  $r, k, t$

$$f = f(r, k, t), \phi = \phi(r, k, t)$$

$\therefore$  The total no. of objects =

$$\iiint f d^3r d^3k = \iiint Q\phi d^3r d^3k$$

The total number of objects is

$$\iiint f d^3r d^3k = \iiint Q\phi d^3r d^3k.$$

The number of objects in  $d^3r$  (concentration) is

$$\int f d^3k = \int Q\phi d^3k.$$

Here it is  $Q = \text{const}$ . In crystals, the integrals are extended over the first Brillouin zone  $B$ . Let

$$\begin{cases} E = E(k_1, k_2, k_3) \\ \alpha = \alpha(k_1, k_2, k_3) \\ \beta = \beta(k_1, k_2, k_3) \end{cases} \quad \begin{cases} k_1 = k_1(E, \alpha, \beta) \\ k_2 = k_2(E, \alpha, \beta) \\ k_3 = k_3(E, \alpha, \beta) \end{cases}$$

$$H(E, \alpha, \beta) = \left[ \frac{\partial(k_1, k_2, k_3)}{\partial(E, \alpha, \beta)} \right]$$

Combined Density of states in  $r & k$

$$Q = \frac{1}{4\pi^3} = \text{Concentration of states in Free Space}$$

we did this in Lecture-3

$$\int f d^3k = \int Q\phi d^3k$$

↳ This thing when integrated in Real space' gives the total no. of objects

we shall deal essential with concentration of Holes & Electrons

→ The integration limits are not specifically marked. but obviously when we are considering a crystal in which all the functions that depend on ' $k$ ' has periodicity of the first

Brillouin zone. we assume Integration over ' $k$ ' must be performed over 1<sup>st</sup>

**Brillouin Zone.**

→ well Integrals of the space are carried Obviously over the volume ' $\underline{W}$ ' of the crystal -

→ Now we perform a change in variables.

$$\boxed{\int f d^3k = \int Q \phi d^3k}$$

It's more convenient to perform integration in terms of Energy than  $k$ .

In order to do so we must change variables and when we go from  $k \rightarrow E$   
we will find Density of states.

→ So far we have considered Density of states only in the Parabolic bands

But it's much of a General Concept. So we will introduce a General form.

→ Change of variables

Here it is  $Q = \text{const}$ . In crystals, the integrals are extended over the first Brillouin zone  $B$ . Let

$$\begin{cases} E = E(k_1, k_2, k_3) \\ \alpha = \alpha(k_1, k_2, k_3) \\ \beta = \beta(k_1, k_2, k_3) \end{cases}$$

$$\begin{cases} k_1 = k_1(E, \alpha, \beta) \\ k_2 = k_2(E, \alpha, \beta) \\ k_3 = k_3(E, \alpha, \beta) \end{cases}$$

New variables  $H(E, \alpha, \beta) = \left[ \frac{\partial(k_1, k_2, k_3)}{\partial(E, \alpha, \beta)} \right]$

$$k_1, k_2, k_3 \rightarrow E, \alpha, \beta$$

$\downarrow$   
Energy

Inverse  
variables  
unspecified  
They could  
be angles

'E' so Integrate Basgto  
నుక్క నుండి

ex:- like change  
from cartesian  
to spherical  
co-ordinates

→ What is important is

$E = E(k_1, k_2, k_3)$  is one of the  
branch of the semiconductor

$$H(E, \alpha, \beta) = \frac{\partial(k_1, k_2, k_3)}{\partial(E, \alpha, \beta)}$$

25°S°29.05°S వాగ్తు

Jacobian

It is denoted with ' $H$ ' because  
 very soon we are gonna consider  
 current density which is denoted by  
 "J"

Electron and Hole Concentration  $\frac{1}{d^3k}$

$$\int Q\Phi d^3k = \int_0^\infty [\iint Q\Phi(E, \alpha, \beta) H(E, \alpha, \beta) d\alpha d\beta] dE$$

$$\int Q\Phi d^3k = \int_{\Delta E_1} + \int_{\Delta E_2} + \dots = n_1 + n_2 + \dots$$

$$n_j(\mathbf{r}, t) = \int_{\Delta E_j} \iint Q\Phi(\mathbf{r}, E, \alpha, \beta, t) H(E, \alpha, \beta) d\alpha d\beta dE$$

$$\gamma(E) \doteq \iint Q H d\alpha d\beta \Rightarrow \int_{\Delta E_j} \gamma(E) dE = n_j(\Phi \equiv 1)$$

It follows that  $\gamma > 0$  is the density of states in  $\mathbf{r}, E$ .

$$P(\mathbf{r}, E, t) \doteq \frac{\iint Q\Phi(\mathbf{r}, E, \alpha, \beta, t) H(E, \alpha, \beta) d\alpha d\beta}{\iint Q H(E, \alpha, \beta) d\alpha d\beta}$$

$$\Rightarrow n_j(\mathbf{r}, t) = \int_{\Delta E_j} \gamma(E) P(\mathbf{r}, E, t) dE$$

Since  $H > 0$  and  $0 \leq \Phi \leq 1$ , it is  $0 \leq P \leq 1$ .  $P$  is the occupation probability in energy. If  $\Phi = \Phi(\mathbf{r}, E, t)$  then  $P = \Phi$ . In equilibrium  $P$  becomes the Fermi statistics  $P = P(\mathbf{r}, E)$ . From  $P = 1 - (1 - P)$  one derives

$$n_j = \int_{\Delta E_j} \gamma dE - \int_{\Delta E_j} \gamma(1 - P) dE = n_j(\Phi \equiv 1) - p_j$$

$$p_j \doteq \int_{\Delta E_j} \gamma(1 - P) dE = \int_{(j)} Q(1 - \Phi) d^3k$$

$\phi(\gamma, E, \alpha, \beta, t) \rightarrow$  It is a function  
depends on  $\gamma, t, E, \alpha, \beta$

$$\int Q\Phi d^3k = \int_0^\infty [\int \int Q\Phi(E, \alpha, \beta) H(E, \alpha, \beta) d\alpha d\beta] dE$$

$$\int Q\Phi d^3k = \int_{\Delta E_1} + \int_{\Delta E_2} + \dots = n_1 + n_2 + \dots$$

First we shall integrate over  $\alpha, \beta$

& integral over  $E$  last.

and the Energy goes from  $0 \rightarrow \infty$

$\rightarrow$  But, if we perform integral over Energy last, we know Energy is split into

Bands.

so, we have lowest Band, Gap & second

Band as so-----

$$\therefore \int Q\phi d^3k = \int_{\Delta E_1} + \int_{\Delta E_2} + \dots = n_1 + n_2 + \dots$$

$$\int_{\Delta E_1} = n_1$$

Integral over 1<sup>st</sup>  
Band by definition  
is the concentration

of electrons of the  
1<sup>st</sup> Band



$$n_j(\mathbf{r}, t) = \int_{\Delta E_j} \iint Q \Phi(\mathbf{r}, E, \alpha, \beta, t) H(E, \alpha, \beta) d\alpha d\beta dE$$

$$\gamma(E) \doteq \iint Q H d\alpha d\beta \Rightarrow \int_{\Delta E_j} \gamma(E) dE = n_j (\Phi \equiv 1)$$

∴ The individual concentration of electrons in single Band is equal to

$$n_j(\mathbf{r}, t) = \int_{\Delta E_j} \left( \iint Q \phi(\mathbf{r}, E, \alpha, \beta, t) H(E, \alpha, \beta) d\alpha d\beta \right) dE$$

→ Let's now consider the situation in which  $\phi=1$  i.e a state is occupied by one electron.

If that is the case then the concentration of electrons is equal to the concentration of the states - because each state is occupied by one electron.

∴ If  $\phi=1$

Revanth Reddy Pannala  
EBIT, Unibo  
ఫోకల్ మెచ్

The integral will transform into

$$\gamma(E) = \iint Q H d\alpha d\beta \quad \rightarrow \text{This integration gives concentration of states.}$$

↓  
combined density of states



awluk gawek  
Band states  
abeli 5g  
2S Band of 5g  
states even

$$\int_{DE_j} \gamma(E) dE = \underline{n_j} (\phi \equiv 1)$$

Total no. of states per unit volume and energy

∴  $\gamma$  is the density of states in

$$\gamma \neq E$$

→ The definition of  $\gamma$  is very general because we did not go through the approximation of parabolic band weight formally took change in variables and defined these density states.

→ we want to now calculate a general case where  $\Phi \neq 1$

& we want to calculate Internal Integral

$$\int Q\Phi d^3k = \int_0^\infty \left[ \iint Q\Phi(E, \alpha, \beta) H(E, \alpha, \beta) d\alpha d\beta \right] dE$$

$$\gamma(E) \doteq \iint Q H d\alpha d\beta \Rightarrow \int_{\Delta E_j} \gamma(E) dE = n_j (\Phi \equiv 1)$$

It follows that  $\gamma > 0$  is the density of states in  $\mathbf{r}, E$ .

$$P(\mathbf{r}, E, t) \doteq \frac{\iint Q\Phi(\mathbf{r}, E, \alpha, \beta, t) H(E, \alpha, \beta) d\alpha d\beta}{\iint Q H(E, \alpha, \beta) d\alpha d\beta}$$

$$\Rightarrow n_j(\mathbf{r}, t) = \int_{\Delta E_j} \gamma(E) P(\mathbf{r}, E, t) dE$$



If we observe the ratio of two integrals

in which  $H$  is positive

$\Phi$  is constant

$\Phi$  is something positive  $0 \leq \Phi \leq 1$

∴ In conclusion the numerator is always

smaller than the denominator and off course  
the fraction can be never negative

$$\iint \Omega \phi(r, E, \alpha, \beta, t) H(E, \alpha, \beta) d\alpha d\beta \\ = p(r, E, t) \cdot \gamma(E)$$

$$\Rightarrow n_j(r, t) = \int_{DE_j} \gamma(E) p(r, E, t) dE$$

we have found that Concentration of  
electrons of Band of index  $j$  can be  
written as Integral over energy of the  
band of the combined density of states  
( $\gamma$ ) multiplied by probability

$p(r, E, t)$  of occupation in energy of  
the state.

→ Doing so we transformed with out

an approximation the calculation from  
 Integration over 'F' to an Integration over  
 energy.

$$0 < P < 1 \quad \text{probability of occupation in Energy}$$

Since  $H > 0$  and  $0 \leq \Phi \leq 1$ , it is  $0 \leq P \leq 1$ .  $P$  is the occupation probability in energy. If  $\Phi = \Phi(\mathbf{r}, E, t)$  then  $P = \Phi$ . In equilibrium  $P$  becomes the Fermi statistics  $P = P(\mathbf{r}, E)$ . From  $P = 1 - (1 - P)$  one derives

$$n_j = \int_{\Delta E_j} \gamma dE - \int_{\Delta E_j} \gamma (1 - P) dE = n_j (\Phi \equiv 1) - p_j$$

$$p_j \doteq \int_{\Delta E_j} \gamma (1 - P) dE = \int_{(j)} Q (1 - \Phi) d^3k$$

$$\begin{aligned} n_j &= \int_{\Delta E_j} \gamma(\mathbf{E}) P(\mathbf{r}, \mathbf{E}, t) dE \\ &\quad \Downarrow \\ &= \int_{\Delta E_j} \gamma P dE \end{aligned}$$

మన లోకాలో  
 ఇరు లోకాలో లోకాలో  
 మాన్య కోట్లు వ్యాపారాలు

$$\Rightarrow \int_{\Delta E_j} \gamma (1 - (1-p) dE$$

$n_j = \int_{\Delta E_j} \gamma dE - \int_{\Delta E_j} \gamma (1-p) dE$

*for  $\phi=1$*

$\therefore$  it is concentration of available states of the Band 'j'

$P_j$

$$P_j = \int_{\Delta E_j} \gamma (1-p) dE$$

Note:- If 'p' is the probability of a state occupied by an Electron then  $1-p$

is the probability of this state non occupied by an Electron.

i.e. probability that the state is Empty.

\* \* \* But an Empty state is a

Hole

$\therefore 1-p$  is the probability of Holes

$$\therefore p_j = \int_{\Delta E_j} \gamma (1-p) dE$$

we get concentration of the Holes

(or) Empty states

I love it

$$p_j \text{ in } 'k' \text{ space} = \int_{(j)} \Omega (1-\phi) d^3 k$$

$$\therefore p_j = \int_{\Delta E_j} \gamma (1-p) dE = \int_{(j)} \Omega (1-\phi) d^3 k$$

Electrons and  $25^{th}$  column  
are ~~empty~~, holes  
~~exists~~  $\Rightarrow$  ~~exists~~  
~~exists~~ -

In ' $k$ ' space it means  
we perform integral  
over ' $k$ '

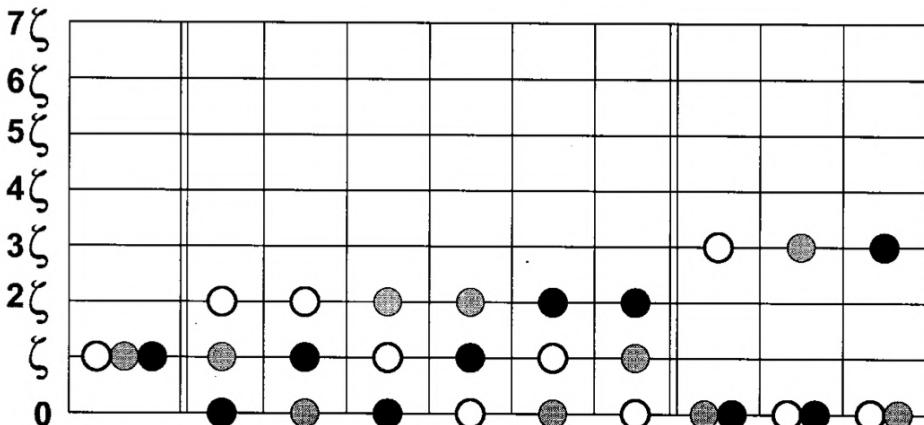
we remember that  $E(k)$  is a many valued function.

→ we should consider only one Branch of index  $j$  in order to count holes belonging to that Branch.

$\rightarrow$  Good Box angle

### Classical particles, Bosons, and Fermions

$$N_s = 3 \quad E_s = 3\zeta$$



C: 1  
B: 1  
F: 0

C: 6  
B: 1  
F: 1

C: 3  
B: 1  
F: 0

→ This page is useful to start an important discussion.

We remember that at some point we defined the structure of Bands of a semiconductor.

The bands are curves over Intervals of energy actually, that represent the possibilities of Energies that can be occupied by electrons in the crystal.

→ Then as a separate subject called Distribution function in general form

which depends on  $\gamma, t, \mathbf{k}$  → momentum  
position time co-ordinates  
co-ordinates

The meaning is that the product of the distribution function times an Elementary Interval  $d^3\gamma d^3k$  gives us no. of particles for instance Electrons that at time 't' belong to that interval.

\* Finding a Distribution Function is a complicated issue if Semiconductors

in Non Equilibrium condition because  
in that case D.F depends on external  
condition applied to the crystal.

→ Instead there is a condition where  
finding D.F is <sup>relatively</sup> easy.

This condition is called THERMODYNAMIC

## EQUILIBRIUM

\* In this case, D.F does not depend on  
Time any more.

But also it can be demonstrated that  
D.F becomes a function that depends only  
on energy.

→ It is implied that in the initial analysis  
we consider a material i.e uniform in space.  
The analysis is subjected to each point in space.  
Later on we see that how the case can  
be extended to material which is not Uniform.

Q

How do the electrons in Equilibrium  
distribute over available Energy  
states ?

Ans  $\omega \approx \frac{E}{\hbar}$  28. Hattalla

The analysis of microscopic particles like electrons must be based on Quantum Mechanics.

→ But let's start our discussion with Classical Mechanics.

We have a system of classical particles for the moment.

These classical particles interact with each other and with the atoms of the crystal.

→ This interaction is essential, if particles do not interact, they do not form a crystal.

→ There is continuous exchange of energy

among particles of a system because of Interaction.

∴ we assume that total system is in **equilibrium**; i.e. The **Total Energy is constant**.

The only thing is that Electrons distribute over possible energies and each individual Electron changes energy after each collision.

→ However, The distribution of Electron in the Energy states is independent of Time. Q What does it mean?

It means that no. of electrons that belong to an Interval of energies does not depend on Time.

The electrons may change, But The total no. of Electron that belongs to an Energy Interval does not change.

→ Given that we must calculate all the

possible ways in which the given no. of electrons can be distributed over energy states.

Because, available states are there as they are given by the Bands and they depend on the property of the crystal.

- It's like we have a no. of Boxes and a certain no. of Balls and we have to find all the possible ways the balls can be distributed into the Boxes.
- This is issue of calculating statistical distribution of particles.
- In the example given below a simple case of Total no. of particles = 3 Available energy states = vertical axis at one equally spaced

# **Classical particles, Bosons, and Fermions**

No. of particles       $N_s = 3$        $E_s = 3\zeta$       Total Energy

Energy Level ( $\zeta$ )	Black Circles	Grey Circles
0	2	1
1	1	1
2	2	1
3	1	1
4	1	0
5	0	1
6	1	0
7	0	1

CAP. 17: STATISTICHE DI EQUILIBRIO

T. 17.9: Possibili distribuzioni di tre particelle formanti un sistema a energia assegnata.

293

The Total energy of particles =  $3T$

- If Energy is represented in horizontal lines and particles with balls the above picture represents All the possible ways the particles can be Distributed among Energy Level for the given total Energy.
- However, in Quantum Mechanics it is not so straight forward as Classical Mechanics because the particles are not distinguishable

we can't distinguish two electrons (so for that matter any particle that) in a system w.r.t. Quantum Mechanics when it comes to similar particles.

i.e. Systems of Identical particles

→ From the figure

For Classical → we have 10 cases possibilities

For Quantum → we have only 3 cases possibilities

(Based on particles being Non-Distinguishable)

→ Even this is not enough because particles must be divided into '2' classes.

I → Class of particles that can be accommodated in same state  
They are called Bosons

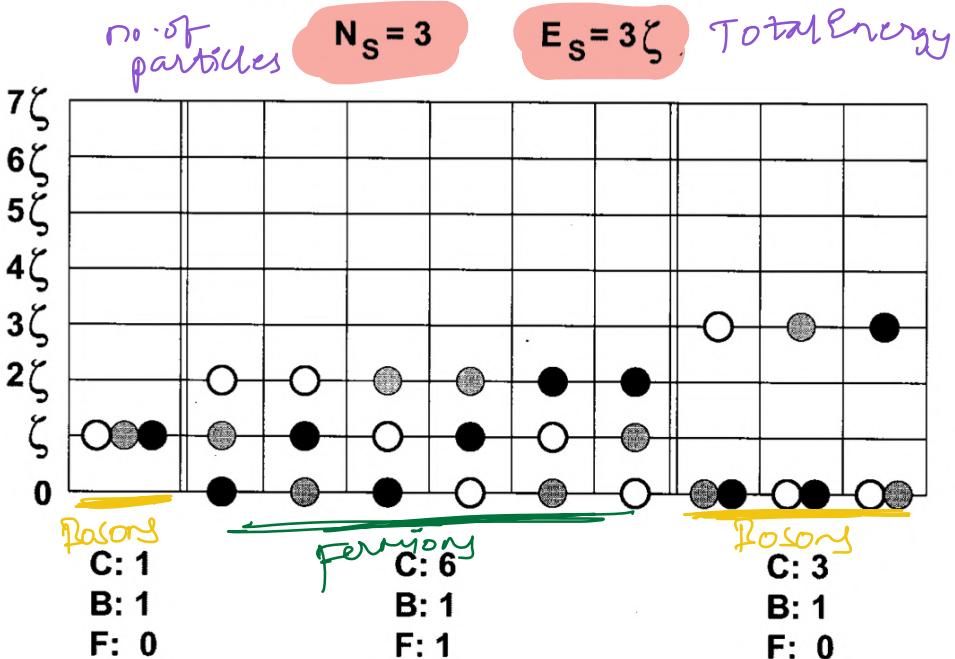
II  $\rightarrow$  Class of Fermions

These particles cannot stay in the same state.

\* When we talk of state we talk of Energy and Spin.

nally

### Classical particles, Bosons, and Fermions



CAP. 17: STATISTICHE DI EQUILIBRIO

T. 17.9: Possibili distribuzioni di tre particelle formanti un sistema a energia assegnata.

293

Conclusion:- when we want to calculate the distribution of the particles into the available energy states first we must use Quantum

Mechanics and 2<sup>nd</sup> year must remember whether we are considering **Bosons** or **Fermions**.

photons are an example of **Bosons**

Electrons are an example of **Fermions**

→ If we know consider a complicated case which has many energy states and many particles and we know these particles are electrons.

we must calculate distribution in Energy in a system of electrons at equilibrium.

The result is

$$P(E) = \frac{1}{\exp[(E - E_F)/k_B T] + 1}$$

This is called  
**Fermi Dirac statistics**

### Equilibrium Statistics for Fermions — III

When the number of energy levels is large and their separation small, the number  $g_i$  of states at energy  $E_i$  can be replaced by the number  $g(E) dE$  of states in the infinitesimal interval  $dE$  around  $E$ . The constraints now read

$$\int_{E_1}^{E_U} \frac{g(E) dE}{\exp(\alpha + \beta E) + 1} = N_S, \quad \int_{E_1}^{E_U} \frac{E g(E) dE}{\exp(\alpha + \beta E) + 1} = E_S,$$

with  $\beta = 1/(k_B T)$ . Consistently,  $N_r$  is replaced with  $N(E) dE$ . The dimensions are  $[g], [N] = \text{J}^{-1}$ . Letting again  $E_F(T) \doteq -k_B T \alpha(T)$ , the expression of  $N$  reads

$$N(E) = g(E) P(E), \quad \text{This is based on QM}$$

where the function

$$P(E) \doteq \frac{1}{\exp[(E - E_F)/(k_B T)] + 1}$$

describes the *Fermi-Dirac statistics*. As  $0 < P(E) < 1$ , this function takes also the meaning of occupation probability of a state at energy  $E$ . If  $E - E_F \gg k_B T$  the probability is approximated by the Maxwell-Boltzmann distribution

$$P(E) \simeq \exp[(E_F - E)/(k_B T)] = P_0 \exp[-E/(k_B T)].$$

This is the approximation is similar to  
the Maxwell - Boltzmann distribution based on  
classical mechanics.

Revanth Reddy Pannala  
EBIT, Unibio  
ఫ్లోట్ బెర్జు

→ The expression is kind of Intuitive

$$P(E) = \frac{1}{\exp((E-E_F)/k_B T) + 1}$$

(i) For High Energies The denominator becomes large and the probability of electron occupying the high energy state is low

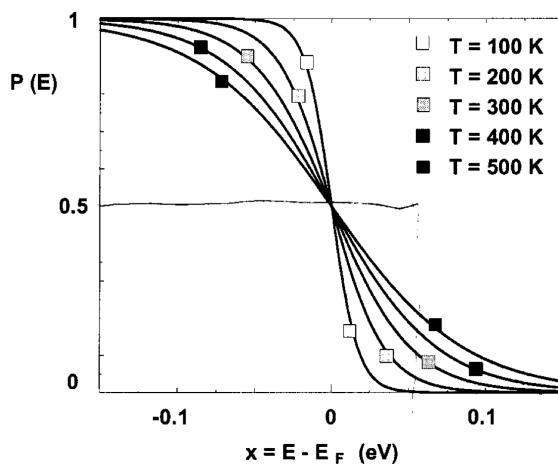
(ii) For  $E = E_F$

The probability =  $\frac{1}{2}$

(iii) For  $E < E_F$

All this illustrated in the Figure Below.

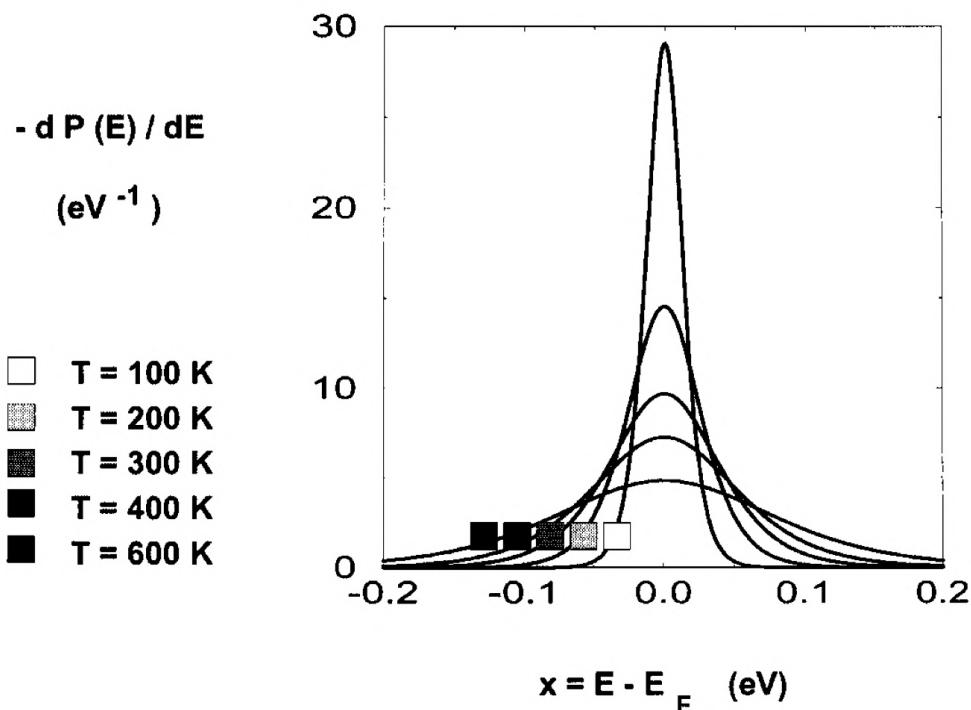
T. 17.13: Andamento della statistica di Fermi-Dirac al variare della temperatura.



$$P(E) = \left\{ \exp [ (E - E_F) / (kT) ] + 1 \right\}^{-1}$$

→ Calculation of Fermi statistics based on Different Temperature

T. 17.14: Derivata della statistica di Fermi-Dirac al variare della temperatura.



→ For Absolute zero  $T = '0' \text{ Kelvin}$

$$P(E) = 1 \quad \text{for } E < E_F$$

$$P(E) = 0 \quad \text{for } E > E_F$$

$$P(E) = \frac{1}{2} \quad \text{for } E = E_F$$

Q What happens to Fermi level when we change Temperature ?

திட்டம் வாயு மூலம் பிரைஸேல்  
ஆக செய்ய...! 😊

Because it can be demonstrated that

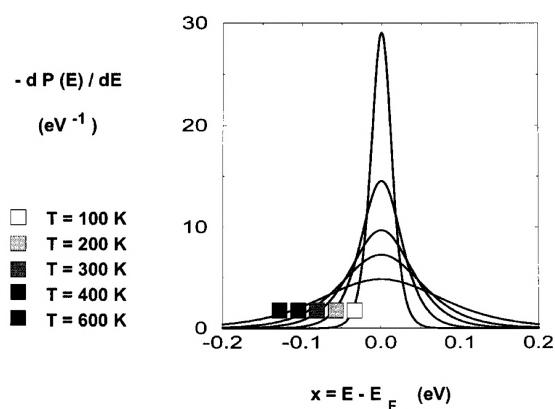
$E_F$  also depends on Temperature.

for practical purpose it's insignificant.

Q How big is the interval for the Fermi statistic probability to go from 0 to 1 ?

திட்டம் வாயு...

T. 17.14: Derivata della statistica di Fermi-Dirac al variare della temperatura.



→ It is of interest to estimate the extension of the region where the main variation of  $P(E)$  occurs. To the purpose, after selecting a number  $\chi_2 < \eta < 1$  define  $E^+$  &  $E^-$  such that

$$P(E^+) = \eta \quad P(E^-) = 1 - \eta$$

It follows

$$\exp\left(\frac{E^+ - E_F}{k_B T_L}\right) = \frac{1-\eta}{\eta}$$

$$\exp\left(\frac{E^- - E_F}{k_B T_L}\right) = \frac{\eta}{1-\eta}$$

$$\therefore E^+ - E^- = 2k_B T_L \log\left(\frac{1-\eta}{\eta}\right)$$

ex:-  $E(p=0.9) - E(p=0.1) = 2k_B T_L \log 9 \cong 4.39 k_B T_L$

$$E(p=0.99) - E(p=0.01) = 2 k_B T_L \log 99$$

$\approx 9.19 k_B T_L$

This is the energy difference for probability to go from almost 1 to 0

Q How big is  $k_B T_L$  ?

We remember that the quantity

$kT/q$  appears in the characteristic of a diode. It is called Thermal Voltage.

$$\frac{kT}{q} = 25 \text{ mV}$$

at Room Temperature

$T_L$  = Lattice Temperature

$\therefore$  for  $p(E) = 0.9$  to  $0.1$

$4 \frac{kT}{q} \approx 100 \text{ mV}$  This is the voltage difference needed for Fermi statistical to go from 0.9 to 0.1 at Room Temperature

→ If repeat the analysis for  
**Bosons**

### Equilibrium Statistics for Bosons — III

When the number of energy levels is large and their separation small, the number  $g_i$  of states at energy  $E_i$  can be replaced by the number  $g(E) dE$  of states in the infinitesimal interval  $dE$  around  $E$ . The constraints now read

$$\int_{E_1}^{E_U} \frac{g(E) dE}{\exp(\alpha + \beta E) - 1} = N_S, \quad \int_{E_1}^{E_U} \frac{E g(E) dE}{\exp(\alpha + \beta E) - 1} = E_S,$$

with  $\beta = 1/(k_B T)$ . Consistently,  $N_r$  is replaced with  $N(E) dE$ .

The dimensions are  $[g], [N] = J^{-1}$ . Letting again  $E_B(T) \doteq -k_B T \alpha(T)$ , the expression of  $N$  reads

$$N(E) = g(E) P(E),$$

where the function

$$P(E) \doteq \frac{1}{\exp[(E - E_B)/(k_B T)] - 1}$$

Here we have  
 a -ve sign

describes the *Bose-Einstein statistics*. As  $P(E)$  may be larger than unity, this function represents the occupation number of a state at energy  $E$ . If  $E - E_B \gg k_B T$  the probability is approximated by the Maxwell-Boltzmann distribution

$$P(E) \simeq \exp[(E_B - E)/(k_B T)] = P_0 \exp[-E/(k_B T)].$$

→ The analysis looks similar to Fermi Dirac statistics but there is a fundamental difference.

- We have a  $\rightarrow$  sign in the denominator  
 $\therefore$  for probability function to be true  
 The exponential function should be High.
- ⇒ The Energy level should be High.

$E_B$  is generally ZERO.

$\therefore$  we also can say that Maxwell Boltzmann case is a limiting factor of both Fermi-Dirac & Bose-Einstein statistic.

- From this analysis we can put there are two big categories of particles

Fermions

Bosons

i) The spin is described by  $\frac{1}{2}$  (Fraction)

e.g:- Electron can have

$$+\frac{1}{2} \text{ or } -\frac{1}{2}$$

The Bosons have the spin that is always described by Integer Number.

ii) For Fermions

For Bosons it is "

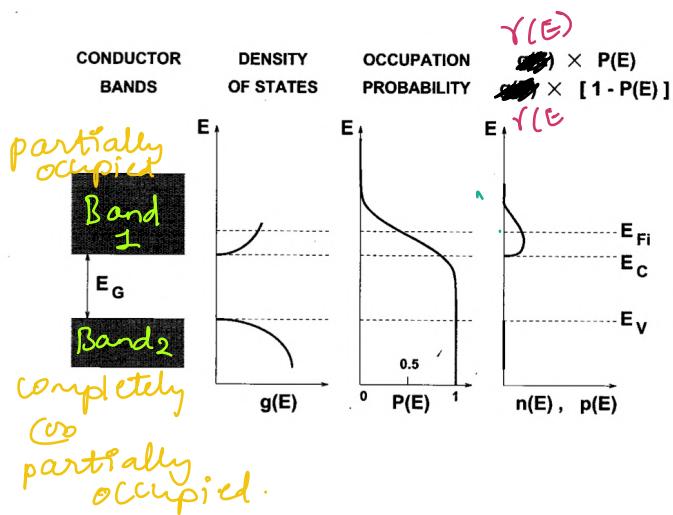
$P(E)$  is always  
between 0 & 1

not necessarily  
between 0 & 1  
it is positive but  
can be larger than  
one.

( $\therefore$  It tells us how  
many Bosons can  
occupy same state)

\* Now we are ready to apply these  
results in the analysis of Distribution of  
Electrons in a crystal in an Equilibrium  
State.

obviously, since we are analysing Electrons  
we use Fermi-Dirac statistics.



T. 22-4: Concentrazione dei portatori nelle bande nel caso di un conduttore.

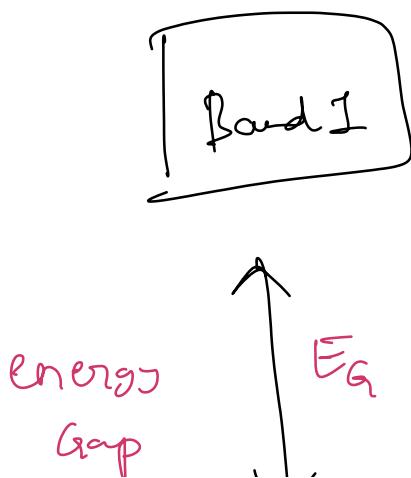
In a crystal we consider almost 2 Bands

Q why do we consider 2 Bands ?

Because Bands that have higher energy are completely empty. So, they have no electrons in them so they cannot contribute to conduction of current.

Also, bands that have lower energy are completely filled and cannot contribute to current. This is not entirely obvious. It must be calculated over oscillators.

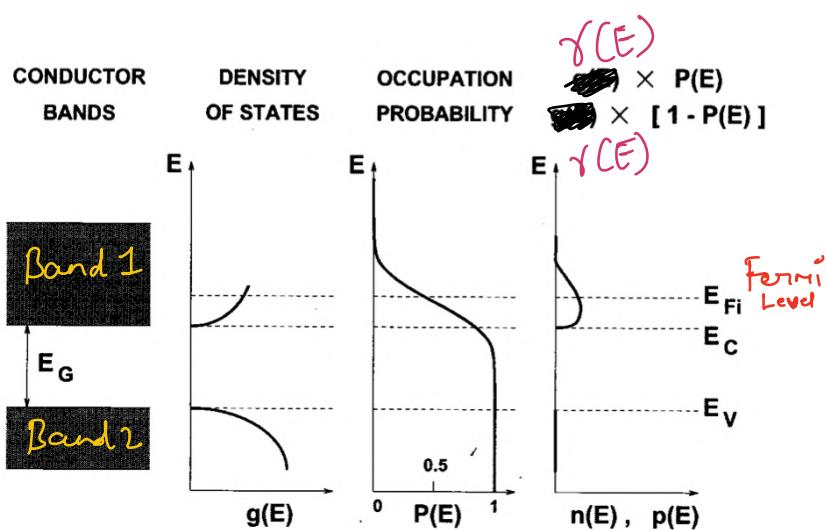
∴ We can say that Bands that are partially occupied by  $e^-$ 's can contribute to the current.



The picture shows schematically  
Two Bands

↓

Band 2



392

T. 22.4: Concentrazione dei portatori nelle bande nel caso di un conduttore.

TAVOLE DI MICROELETTRONICA

**Band 1:** It's assumed to be a band that is partially occupied by electrons.

**Band 2:** It's assumed to be occupied completely or partially.

The Energy Interval between Band 1 and Band 2 is called Energy Gap. ( $E_G$ )

→ we have another parameter at our disposal called **Fermi statistics** and we see that Fermi statistics has one parameter in it.

We are considering a system at equilibrium, so the temperature is given (prescribed)

↳ we remember that given the **Temperature** the value of the **Fermi Level** is also prescribed (which is an Energy).

→ In the graph the **Vertical axis** is **ENERGY axis**.

one of the possible energies on the vertical axis is equal to **Fermi Energy**

It is intuitive that there are only two possibilities for the **Fermi level**

(i) One possibility is that the Fermi level is in one of the bands.

- (ii) The other possibility is that Fermi level is in one of the gaps.
- (iii) There is also a possibility that Fermi level is located exactly to the edge of a Band. We shall not consider this case.

→ In the Figure we are analysing the Fermi Level  $E_F$ . It is inside a band. So when the Fermi level is inside a band we call that a Conduction Band. and the band that is immediately below it we call it valence band.

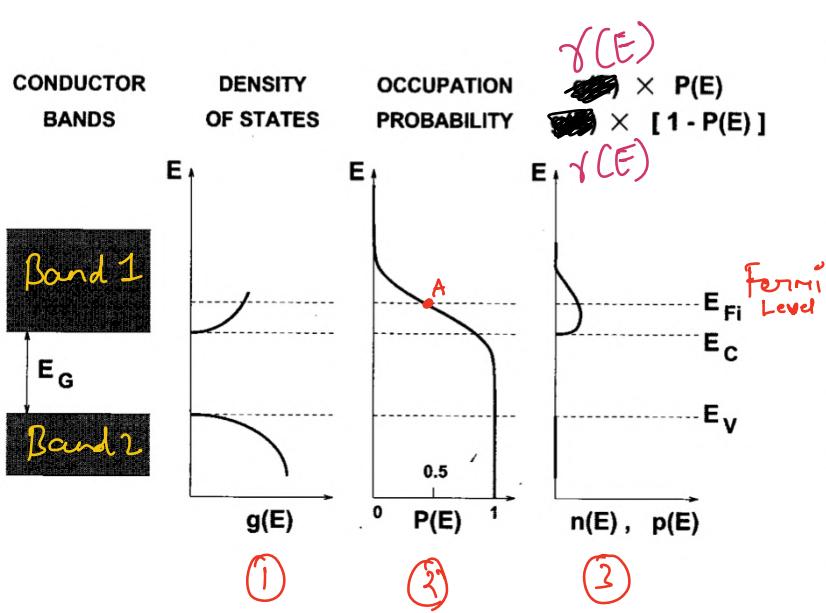
→  Here we assume a pure crystal i.e. intrinsic crystal

ఇంద్రు అంగ రావుకుంటాఏ, My God...!

ఈ Topic నుండి మధ్యాలైనిది...!

electron ను Energy state లో ఉంటు, ఫోన్ ఎంబు  
చెప్పుకొను రాని, అని అంత ఎండె తెల్గు

క్రాంతులన్ను, అది మధ్యంగ వుండు  
వర్షాల గోడి మాటల లీటు నిఱణి ఉపాధి.



T. 22.4: Concentrazione dei portatori nelle bande nel caso di un conduttore.

A: If fermi level belongs to a band  
as we see in the figure the point A  
is where the fermi statistic is  $\frac{1}{2}$

Figures

①, ②, ③ are different graphs representing  
Density of states, Occupation probability &

→ Fig. ① states that the probability of occupation  
of the state of the band that are beyond

Fermi level is small. i.e there are many empty states in the upper part of the Band I.

The probability of occupation of energy states that are below Fermi level is large and will go to 1 gradually.

\* \* The important thing is we see that in

Fig ① the Fermi statistics is already practically equal to 1 in the Forbidden Gap.

So when we go into the Valance Band

The Fermi statistics is equal to ONE.

That means all states are occupied.

(or) If we want to consider holes the probability of there is a hole is

$$1 - p(E) = 0$$

$$\therefore p(E) = 1 \text{ (In Valance Band)}$$

we remember that a Band i.e Completely Filled does not contribute to the current.

$\therefore$  valance Band does not contribute to current.

→ we also see that above the conduction band there are infinitely many bands but they are empty. Because Fermi statistics is almost equal to ZERO in the upper part of the conduction band.

In conclusion, in a case when Fermi level belongs to a band, only that band contributes to current. This is typical situation of a crystal i.e. a Conductors.

Ex:- Metals

& quantity of electrons available for conduction is generally large and this explains why conductors have large conductivity.

Q How can we calculate, qualitatively at least the concentration of e<sup>-</sup>'s of the conduction band ?

We have to take Density of States N(E)

then we multiply Density of states by  
Fermi statistics and Finally we integrate  
over the Energies.

Q How do we describe density of states ?

We have already derived density of states  
using parabolic Band approximation.

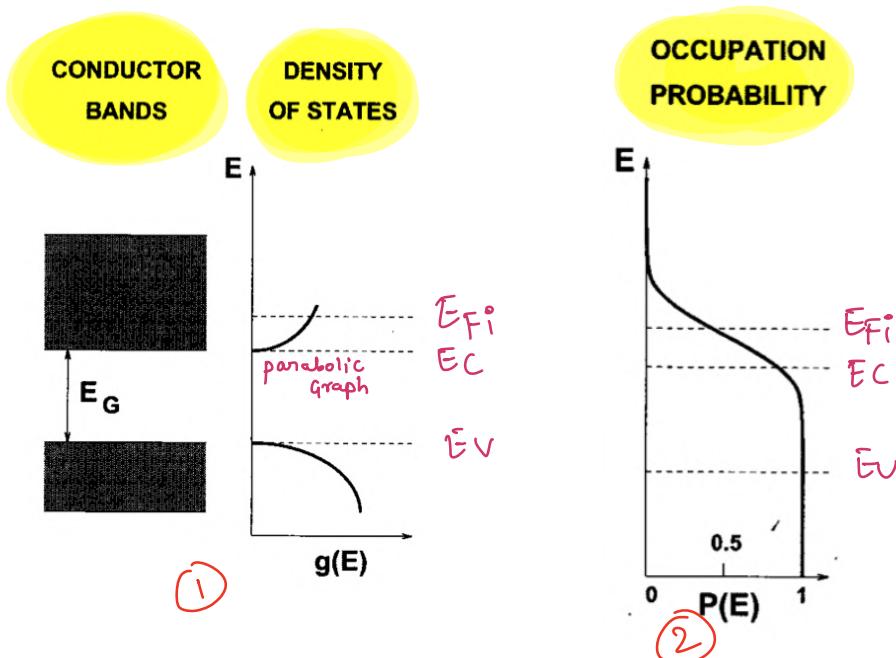
The parabolic Band approximation applies  
if we consider the portion of the Band .

i.e actually near the Minimum of the Band .

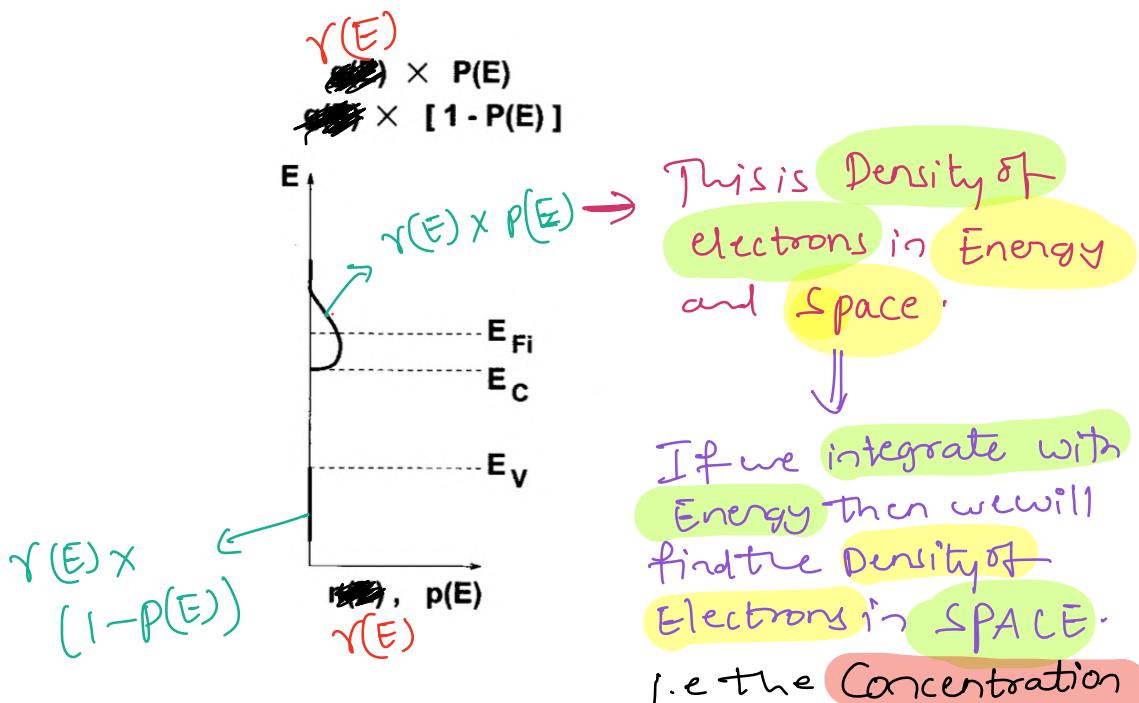
But, we can do this because, when we  
observe Fermi statistics , it tells us that  
the probability of occupation is largest at  
the Minimum

So, we can apply parabolic Band approximation.  
When we adopt it the Density of states in  
3D is like  $\sqrt{E}$ .

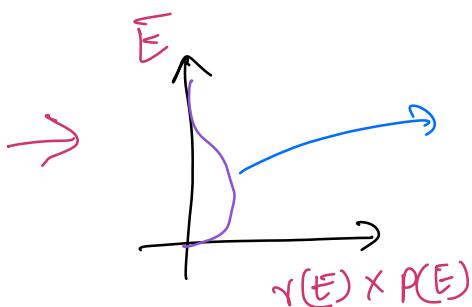
i.e if we look at Graph E (vs) Density of  
states  $\gamma(E)$



→ Considering the conduction Band, we know that we multiply  $\gamma(E) \times p(E)$   
i.e multiplying Both we get the Fig ② shown below.



This is the Quantity we are seeking for.



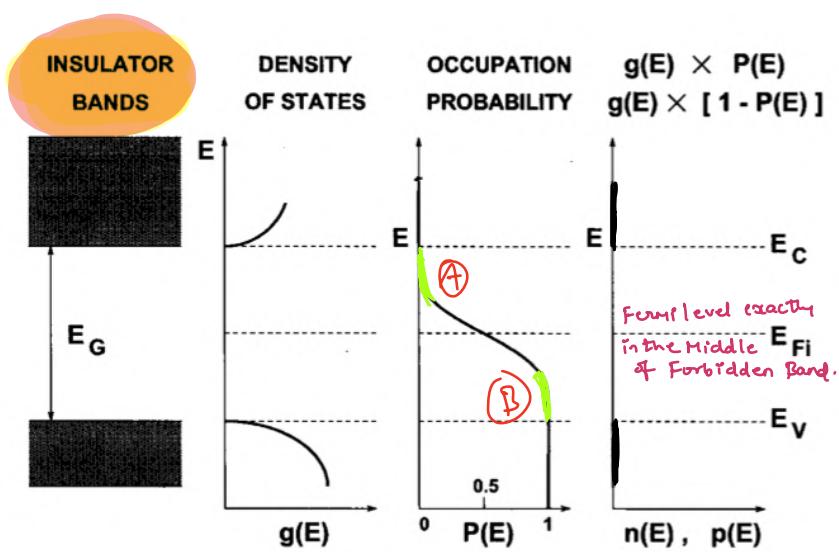
Integral of this curve in Energy is nothing else than Area of this Function  $(r(E) \times P(E))$  w.r.t to the Energy axis. in the Conduction Band.

→ In order to find the calculate the concentration of Holes in the valance Band we can do the same.

i.e Integrate the curve  $\frac{r(E) \times (1 - P(E))}{\text{w.r.t Energy}}$   
But this term is zero.

\* When Fermi Level is in the Forbidden Gap and assume that the Gap is too large

T. 22.5: Concentrazione dei portatori nelle bande nel caso di un isolante.



Fermi statistics goes from practically 1

to 0 in a smaller range of energies  
 If Energy Gap is Large  
 → we can see that Fermi statistics go to zero  
 at A when we are still in the Forbidden Gap and  
 at B it goes to ONE when we are still in  
 the Forbidden Gap.

In conclusion; when we eventually go  
 up in Energy and enter the upper Band the  
 probability is ZERO. So the concentration  
 of electrons is zero. because we will

take product of  $\gamma(E)$  &  $P(E)$

\* Upper Band is Completely Empty.

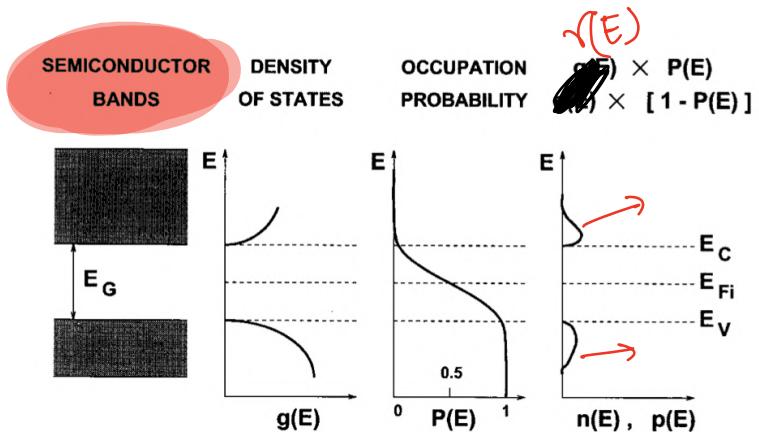
\* Lower Band is Completely Empty.

So, all Bands are either Completely empty or Completely filled.

\* This type of Crystal is an

Insulator.

\* There is also another case which is possible i.e. Fermilevel is in Forbidden Gap but Energy Gap is small. Semiconductor



Both are  
Non  
ZERO.

$\therefore$  we have Non zero concentration of  
Electron in C.B & Non zero concentration  
of holes in Valence Band.

This is called Semiconductor.

→ Now we will go ahead and calculate  
The concentration of Electrons and Holes in  
Semiconductors - by introducing New

Mathematical Functions

The First important function we are gonna  
introduce is Euler's Gamma Function.

$$T(n) = \int_0^{\infty} x^{n-1} \exp(-x) dx$$

' $n$ ' can be a complex number.  
and should be positive

T. 22.7: Definizione e alcune proprietà degl'integrali di Fermi.

Fermi Integrals

## Euler's Gamma function

$$\Gamma(\lambda) \doteq \int_0^{+\infty} x^{\lambda-1} \exp(-x) dx, \quad \Re(\lambda) > 0$$

$$\Gamma(1) = 1, \quad \Gamma(\lambda + 1) = \lambda \Gamma(\lambda), \quad \Gamma(n+1) = n \Gamma(n) = \dots = n!$$

$$\Gamma(1/2) = \sqrt{\pi}, \quad \Gamma(3/2) = (1/2) \Gamma(1/2) = \sqrt{\pi}/2, \quad \dots \downarrow$$

Fermi integral of order  $\alpha$ 

Recursive Relation  
Integration by parts

$$\Phi_\alpha(\xi) \doteq \frac{1}{\Gamma(\alpha+1)} \int_0^\infty \frac{x^\alpha}{\exp(x-\xi)+1} dx, \quad \alpha > -1$$

$$\frac{d\Phi_\alpha}{d\xi} = \Phi_{\alpha-1}, \quad \frac{\Phi_{\alpha-1}}{\Phi_\alpha} = \frac{d \log \Phi_\alpha}{d\xi}, \quad \alpha > 0$$

$$\Phi_{1/2}(\xi) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2}}{\exp(x-\xi)+1} dx$$

$$\Phi_{1/2}(\xi) \simeq \begin{cases} \exp(\xi) & -\infty < \xi < -1 \\ [\exp(-\xi) + 1/4]^{-1} & -1 < \xi < 5 \\ 4\xi^{3/2}/(3\sqrt{\pi}) & 5 < \xi < +\infty \end{cases}$$

Special cases

Using these special mathematical functions

Fermi Integral of order  $\lambda$  and

Euler's Gamma function we can calculate the electron concentration in an Intrinsic crystal.

## Intrinsic Concentration — I

Intrinsic semiconductor at equilibrium

$$\text{Intrinsic Electron Concentration } n_i \doteq \frac{N_e}{\Omega}, \quad p_i \doteq \frac{N_h}{\Omega} \quad \begin{matrix} \text{Total no. of} \\ \text{electrons} \end{matrix} \quad \begin{matrix} \text{Intrinsic Hole} \\ \text{concentration} \end{matrix}$$

$\Omega$  volume of crystal

$$P = \frac{1}{\exp[(E - E_{Fi})/(k_B T_L)] + 1}, \quad k_B = 1.38 \times 10^{-23} \text{ J/K}$$

Boltzmann's Constant

$$N_e = \int_{E_C}^{E_{CU}} g(E) P(E) dE, \quad N_h = \int_{E_{VL}}^{E_V} g(E) [1 - P(E)] dE$$

$$T_L \rightarrow 0 : P \rightarrow \begin{cases} 1 & E < E_{Fi} \\ 0 & E > E_{Fi} \end{cases} \Rightarrow N_e = N_h \quad \forall T_L \Rightarrow E_{Fi}(T_L)$$

$$E_C < E < E_{CU} : E - E_{Fi} = \underbrace{E - E_C}_{E_e > 0} + \underbrace{E_C - E_{Fi}}_{\zeta_e}$$

$$E_{VL} < E < E_V : E_{Fi} - E = \underbrace{E_{Fi} - E_V}_{\zeta_h} + \underbrace{E_V - E}_{E_h > 0}$$

$$P(\lambda) = \frac{1}{\exp(\lambda) + 1} \implies 1 - P(\lambda) = \frac{1}{\exp(-\lambda) + 1}$$

$$\Phi_\alpha(\xi) \doteq \frac{1}{\Gamma(\alpha + 1)} \int_0^\infty \frac{x^\alpha}{\exp(x - \xi) + 1} dx, \quad \alpha > -1$$

→ since it's Intrinsic Semiconductor

$$n_i = \frac{N_e}{V} \rightarrow \begin{matrix} \text{Total no. of electrons in the crystal} \\ \text{in Conduction Band} \end{matrix}$$

$\rightarrow$  volume of the crystal

$$P_i = \frac{N_h}{V} \rightarrow \begin{matrix} \text{Total no. of holes in the valence} \\ \text{Band} \end{matrix}$$

$$P = \frac{1}{\exp[(E - E_{F_i})/(k_B T_L)] + 1}, \quad k_B = 1.38 \times 10^{-23} \text{ J/K}$$

Boltzmann's Constant

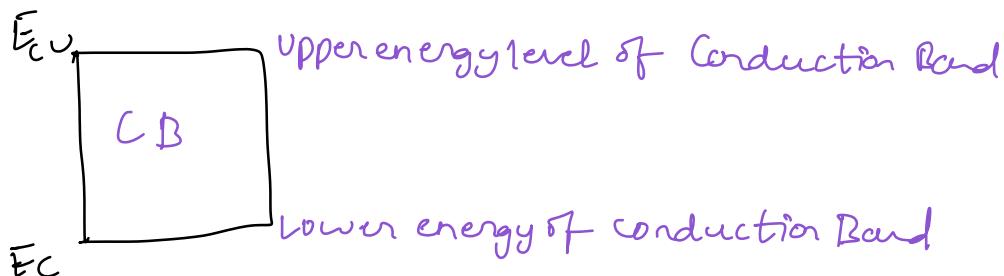
$$N_e = \int_{E_C}^{E_{CU}} f(E) P(E) dE, \quad N_h = \int_{E_{VL}}^{E_V} f(E) [1 - P(E)] dE$$

↓

Total no. of electrons in  
conduction Band

Density  
of states

probability  
of hole



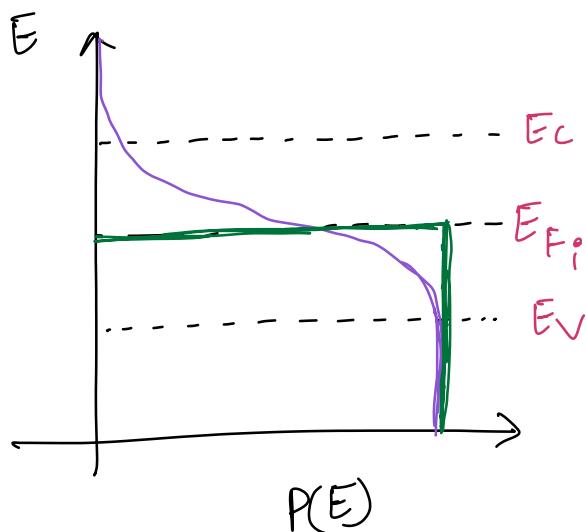
→ Before proceeding with the calculation of

no. of Electrons & Holes. we must make an observation regarding as in

Do we expect any relation b/w no. of electrons in Conduction Band & No. of holes in Valence Band.

→ ∴ in order to seek relation b/w  $N_e$  &  $N_h$  we do this reasoning, we start at a temperature of  $0^\circ K$

At  $0^\circ K$



- Fermi statistic Electron distribution at  $0^\circ K$
- Normal Fermi statistic distribution at Room Temperature

∴ at  $0^\circ K$  There will be **No electrons** in CB  
at **No holes** in the VB.

→ Assume we start ↑ Temperature, Of course

we go through Equilibrium state. i.e  
we increase the Temperature Very very  
slowly.

- we provide energy to the crystal Externally.  
This external energy is taken by atoms and  
some of it is taken by the electrons and  
at some point the electron will have  
<sup>enough Energy</sup> to acquire to make a Transition from  
Valence Band to Conduction Band.
- So, that there is one electron in CB  
and an empty state in VB which is called  
Hole.
- And Eventually at Room Temperature  
the total no. of electrons are equal to  
Total no. of holes in the Valence Band.

In conclusion

$$N_e = N_h$$

( $\because$  we assumed the material  
is uniform with out any defects)

$N_e$  &  $N_h$  can be calculated using

$$N_e = \int_{E_C}^{E_{CU}} \gamma(E) P(E) dE$$

$$N_h = \int_{E_{VL}}^{E_V} \gamma(E) (1 - P(E)) dE$$

In order to calculate two integrals it is convenient to change the **Integration Variable**

\* ~~Want to change variables & make the limits ... !~~

$$N_e = \int_{E_C}^{E_{CU}} g(E) P(E) dE, \quad N_h = \int_{E_{VL}}^{E_V} g(E) [1 - P(E)] dE$$

$$T_L \rightarrow 0 : P \rightarrow \begin{cases} 1 & E < E_{Fi} \\ 0 & E > E_{Fi} \end{cases} \Rightarrow N_e = N_h \quad \forall T_L \Rightarrow E_{Fi}(T_L)$$

This is true

$$E_C < E < E_{CU} : E - E_{Fi} = \underbrace{E - E_C}_{E_e > 0} + \underbrace{E_C - E_{Fi}}_{\xi_e}$$

$$E_{VL} < E < E_V : E_{Fi} - E = \underbrace{E_{Fi} - E_V}_{\xi_h} + \underbrace{E_V - E}_{E_h > 0}$$

$\xi_e, \xi_h$  we will calculate about this  
in future it is related to  
Fermilevel.

↑ Here 'd' has nothing to do with that of Gamma function

$$P(\lambda) = \frac{1}{\exp(\lambda) + 1} \implies 1 - P(\lambda) = \frac{1}{\exp(-\lambda) + 1}$$

$$\Phi_\alpha(\xi) \doteq \frac{1}{\Gamma(\alpha + 1)} \int_0^\infty \frac{x^\alpha}{\exp(x - \xi) + 1} dx, \quad \alpha > -1$$

## Intrinsic Concentration — II

Electrons in the conduction band

$$E_C < E < E_{CU} : \quad g(E) \simeq \Omega \frac{\sqrt{2}}{\pi^2 \hbar^3} M_C m_e^{3/2} \sqrt{E - E_C}$$

$$n_i = \frac{N_e}{\Omega} \simeq \frac{\sqrt{2}}{\pi^2 \hbar^3} M_C m_e^{3/2} \int_{E_C}^{+\infty} \frac{\sqrt{E - E_C}}{\exp[(E - E_F)/k_B T_L] + 1} dE$$

$$n_i = \frac{\sqrt{2}}{\pi^2 \hbar^3} M_C m_e^{3/2} \int_0^{+\infty} \frac{\sqrt{E_e}}{\exp[(E_e + \zeta_e)/(k_B T_L)] + 1} dE_e$$

$$x = E_e/(k_B T_L), \quad \xi_e = -\zeta_e/(k_B T_L)$$

Fermi Integral

$$n_i = \frac{\sqrt{2}}{\pi^2 \hbar^3} M_C m_e^{3/2} (k_B T_L)^{3/2} \int_0^{+\infty} \frac{\sqrt{x}}{\exp(x - \xi_e) + 1} dx$$

$$n_i = \left[ \frac{\sqrt{2}}{\pi^2 \hbar^3} M_C m_e^{3/2} (k_B T_L)^{3/2} \frac{\sqrt{\pi}}{2} \right] \Phi_{1/2}(\xi_e)$$

$$n_i = N_C \Phi_{1/2}(\xi_e),$$

$$N_C \doteq 2M_C \left( \frac{m_e}{2\pi \hbar^2} k_B T_L \right)^{3/2}$$

Effective density of states of the conduction band.

$$\xi_e = -\beta_e / k_B T_L$$



### Intrinsic Concentration — III

Holes in the valence band

$$E_{VL} < E < E_V : \quad g(E) \simeq \Omega \frac{\sqrt{2}}{\pi^2 \hbar^3} M_V m_h^{3/2} \sqrt{E_V - E}$$

$$p_i = \frac{N_h}{\Omega} \simeq \frac{\sqrt{2}}{\pi^2 \hbar^3} M_V m_h^{3/2} \int_{-\infty}^{E_V} \frac{\sqrt{E_V - E}}{\exp[(E_{F_i} - E)/(k_B T_L)] + 1} dE$$

$$p_i = \frac{\sqrt{2}}{\pi^2 \hbar^3} M_V m_h^{3/2} \int_0^{+\infty} \frac{\sqrt{E_h}}{\exp[(E_h + \zeta_h)/(k_B T_L)] + 1} dE_h$$

$$x = E_h/(k_B T_L), \quad \xi_h = -\zeta_h/(k_B T_L)$$

$$p_i = \frac{\sqrt{2}}{\pi^2 \hbar^3} M_V m_h^{3/2} (k_B T_L)^{3/2} \int_0^{+\infty} \frac{\sqrt{x}}{\exp(x - \xi_h) + 1} dx$$

$$p_i = \frac{\sqrt{2}}{\pi^2 \hbar^3} M_V m_h^{3/2} (k_B T_L)^{3/2} \frac{\sqrt{\pi}}{2} \Phi_{1/2}(\xi_h)$$

Fermi Integral

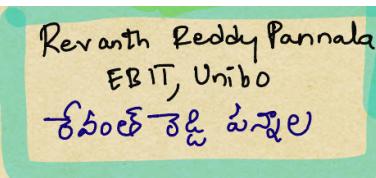
$$p_i = N_V \Phi_{1/2}(\xi_h), \quad N_V \doteq 2M_V \left( \frac{m_h}{2\pi \hbar^2} k_B T_L \right)^{3/2}$$

$T_e$  &  $T_h$  depend on Fermi Level  
which is dealt in the coming lessons  
but for now we can say that

$$\left. \begin{array}{l} p_i = N_v \phi_{1/2}(E_h) \\ n_i = N_c \phi_{1/2}(E_e) \end{array} \right\} \text{Both depend on Fermi level.}$$

Exam Question: How do we determine the Fermi Level ?

Ans: Twisted Q.



It can be  
calculated  
independently

## Intrinsic Concentration — IV

Energy  
gap

$$-(\xi_e + \xi_h) = \frac{\zeta_e + \zeta_h}{k_B T_L} = \frac{E_C - E_{F_i} + E_{F_i} - E_V}{k_B T_L} = \frac{E_G(T_L)}{k_B T_L}$$

*n<sub>i</sub> = p<sub>i</sub>*  $\implies M_C m_e^{3/2} \Phi_{1/2}(\xi_e) = M_V m_h^{3/2} \Phi_{1/2}(\xi_h)$

*Intrinsic Semiconductor* *This relation is OK. But not enough because it involves ξ<sub>e</sub> & ξ<sub>h</sub>*

$$\implies \xi_e \approx \xi_h, \quad \zeta_e \approx \zeta_h \approx E_G/2 > 0$$

*T<sub>L</sub> ~ 300 K : E<sub>G</sub> ≫ k<sub>B</sub>T<sub>L</sub>, -ξ<sub>e</sub> ≪ 1, -ξ<sub>h</sub> ≪ 1*

$$-\xi \gg 1 : \Phi_{1/2}(\xi) \simeq \frac{2 \exp(\xi)}{\sqrt{\pi}} \int_0^{+\infty} \sqrt{x} \exp(-x) dx = \exp(\xi)$$

$$n_i \simeq N_C \exp(\xi_e) = N_C \exp[-(E_C - E_{F_i})/(k_B T_L)]$$

$$p_i \simeq N_V \exp(\xi_h) = N_V \exp[-(E_{F_i} - E_V)/(k_B T_L)]$$

$$n_i p_i = n_i^2 \simeq N_C N_V \exp(\xi_e + \xi_h) = N_C N_V \exp[-E_G/(k_B T_L)]$$

$$N_C N_V = \frac{M_C M_V}{2\pi^3 \hbar^6} (m_e m_h)^{3/2} (k_B T_L)^3$$

$$E_G(T_L) \approx E_{G0} - \alpha T_L^2 / (T_L + \beta)$$



$$-(\xi_e + \xi_h) = \frac{\zeta_e + \zeta_h}{k_B T_L} = \frac{E_C - E_{F_i} + E_{F_i} - E_V}{k_B T_L} = \frac{E_G(T_L)}{k_B T_L} \quad \textcircled{1}$$

$$n_i = p_i \implies M_C m_e^{3/2} \Phi_{1/2}(\xi_e) = M_V m_h^{3/2} \Phi_{1/2}(\xi_h) \quad \textcircled{2}$$

Here we have two relations ① & ②

② involves Fermi Integrals which are not easy to deal with

So, the only way possible is to calculate numerically the two values of  $\mathcal{F}_e, \mathcal{F}_h$  and then we calculate  $T_e, T_h$  and eventually will calculate the difference.

$$T_e = E_C - E_{F_i}, T_h = E_F - E_V$$

In the intrinsic case we can make an estimate i.e

For silicon

$$\gamma_i = p_i \Rightarrow$$

$$M_C m_e^{3/2} \phi_2(E_e) \\ = M_V m_h^{3/2} \phi_2(E_h)$$

$$M_C \approx 6, M_V = 2$$

$|m_h| \approx$  we can say somehow compensates for

$$\left(\frac{1}{m_e}\right)$$

$$(M_C = 3M_V)$$

So just for estimate

$$M_C m_e^{\gamma_2} \approx M_V m_h^{\gamma_2}$$

Then we are left with

$$\boxed{\phi_{\gamma_2}(E_e) \equiv \phi_{\gamma_2}(E_{e_h})}$$

Fermi integral is monotonic function  
ever increasing function  
of the Argument

$$\frac{d\phi_\alpha}{dE} = \phi_{\alpha-1}$$

This is true  
implies

$\phi_\alpha$  is monotonic  
ever increasing function

## Intrinsic Concentration — IV

$$-(\xi_e + \xi_h) = \frac{\zeta_e + \zeta_h}{k_B T_L} = \frac{E_C - E_{F_i} + E_{F_i} - E_V}{k_B T_L} = \frac{E_G(T_L)}{k_B T_L} \quad (1)$$

$$n_i = p_i \implies M_C m_e^{3/2} \Phi_{1/2}(\xi_e) = M_V m_h^{3/2} \Phi_{1/2}(\xi_h)$$

$$\implies \xi_e \simeq \xi_h, \quad \zeta_e \simeq \zeta_h \simeq E_G/2 > 0$$

$$T_L \sim 300 \text{ K} : \quad E_G \gg k_B T_L, \quad -\xi_e \gg 1, \quad -\xi_h \gg 1$$

$$-\xi \gg 1 : \boxed{\Phi_{1/2}(\xi) \simeq \frac{2 \exp(\xi)}{\sqrt{\pi}} \int_0^{+\infty} \sqrt{x} \exp(-x) dx = \exp(\xi)}$$

All became Fermi integral approximation to exponential.

$$n_i \simeq N_C \exp(\xi_e) = N_C \exp[-(E_C - E_{F_i})/(k_B T_L)]$$

$$p_i \simeq N_V \exp(\xi_h) = N_V \exp[-(E_{F_i} - E_V)/(k_B T_L)]$$

$$n_i p_i = n_i^2 \simeq N_C N_V \exp(\xi_e + \xi_h) = N_C N_V \exp[-E_G/(k_B T_L)]$$

product of equilibrium concentration

$$N_C N_V = \frac{M_C M_V}{2\pi^3 \hbar^6} (m_e m_h)^{3/2} (k_B T_L)^3$$

$$E_G(T_L) \approx E_{G0} - \alpha T_L^2 / (T_L + \beta)$$

They have nothing to do with symbols in Fermi statistics  
 $\alpha, \beta$  are free

Energy Gap  $E_G$  also depends on Temperature.

## Intrinsic Concentration — V

$$E_G \gg k_B T_L$$

$$n_i \simeq \sqrt{N_C N_V} \exp[-E_G/(2k_B T_L)]$$

effectively  
it electron  
hole

	$E_{G0}$ (eV)	$\alpha$ (eV/K)	$\beta$ (K)	$E_G(T_a)$	$m_e/m_0$	$m_h/m_0$
Ge	0.747	4.77	235	0.66	0.22	0.31
Si	1.170	4.73	636	1.12	0.33	0.56
GaAs	1.519	5.41	204	1.43	0.68	0.50

Room Temperature

	$N_C(T_a)$ (cm <sup>-3</sup> )	$N_V(T_a)$ (cm <sup>-3</sup> )	$n_i(T_a)$ (cm <sup>-3</sup> )
Ge	$1.04 \times 10^{19}$	$0.43 \times 10^{19}$	$1.39 \times 10^{12}$
Si	$2.82 \times 10^{19}$	$1.05 \times 10^{19}$	$7.61 \times 10^9$
GaAs	$4.45 \times 10^{19}$	$0.99 \times 10^{19}$	$2.40 \times 10^6$

$$n_i = p_i \implies M_C m_e^{3/2} \exp(\xi_e) \simeq M_V m_h^{3/2} \exp(\xi_h)$$

$$\xi_h - \xi_e = \xi_h + \xi_q - 2\xi_e \simeq \log[M_C m_e^{3/2} / (M_V m_h^{3/2})]$$

$$E_C - E_{F_i} \simeq E_G/2 + (k_B T_L/2) \log[M_C m_e^{3/2} / (M_V m_h^{3/2})]$$

The large differences in the Intrinsic carrier of  
Li, Ge, GaAs despite  $N_C, N_V$  being in almost the same order

This is because of exponential of  $E_G$

$\therefore$  A small difference in  $E_G$  will contribute

a lot to the intrinsic concentration of electrons.

- Intrinsic concentration of Ge is high at Room Temperature compared to Si & GaAs.  
we remember that
- One of -ve aspects of Ge is intrinsic concentration  $\text{at equilibrium}$  is large, which is why we have large loss in the reverse current of PN Junction made of Ge.

→ Now, we made an estimate in order to make easy calculation of the fermilevel and the estimate has led to the conclusion that we can use the exponentials instead of Fermi Integrals when we calculate the Intrinsic calculation.

→ At this point we can improve the calculation.

#### Intrinsic Concentration — IV

$$-(\xi_e + \xi_h) = \frac{\zeta_e + \zeta_h}{k_B T_L} = \frac{E_C - E_{F_i} + E_{F_i} - E_V}{k_B T_L} = \frac{E_G(T_L)}{k_B T_L}$$

$$n_i = p_i \implies M_C m_e^{3/2} \Phi_{1/2}(\xi_e) = M_V m_h^{3/2} \Phi_{1/2}(\xi_h)$$

Since we already know these two Fermi Integrals can be replaced with exponentials

Then we can repeat the calculation without neglecting the coefficients i.e. without assuming that  $M_C m_e^{3/2} \approx M_V m_h^{3/2}$  are equal.

We simply keep the coefficients and put the exponentials into place of Fermi Integrals.

$$n_i = p_i \implies M_C m_e^{3/2} \exp(\xi_e) \simeq M_V m_h^{3/2} \exp(\xi_h)$$

$$\xi_h - \xi_e = \xi_h + \xi_q - 2\xi_e \simeq \log[M_C m_e^{3/2} / (M_V m_h^{3/2})]$$

$$E_C - E_{F_i} \simeq E_G/2 + (k_B T_L/2) \log[M_C m_e^{3/2} / (M_V m_h^{3/2})]$$

This is a very small quantity

Because  $\log \left[ \frac{M_C m_e^{3/2}}{M_V m_h^{3/2}} \right] \approx 0$

This quantity is almost equal

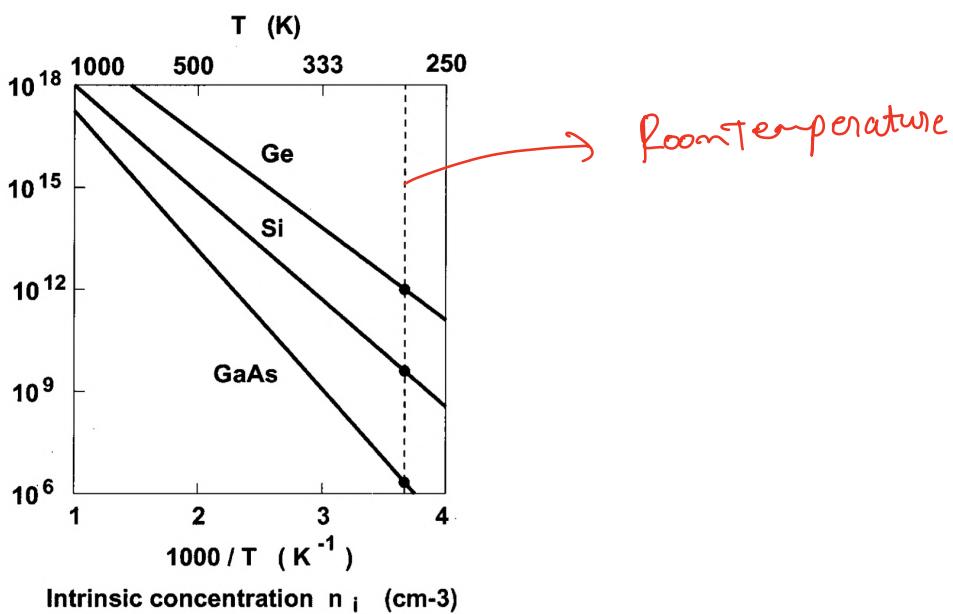
to one.

→ When we want to represent in Graphic form the dependence of Intrinsic carrier Concentration on Temperature, we should express the equation in a diagram

$$n_i \approx \sqrt{N_C N_V} \exp \left[ -E_G / 2k_B T_L \right]$$

We take **log** of the equation, to simplify the plotting on a graph.

T. 22.13: Grafico di Arrhenius della concentrazione intrinseca per Ge, Si e GaAs.



\* Here in the graph if we increase the Temperature we move to the left.

\*\* In some books The intrinsic carrier concentration of silicon at room temperature instead of  $7.61 \times 10^9$  is

$1.45 \times 10^{10}$  (They might have used slightly different value for Room Temperature)

→ So, far we have considered diagrams that represent Energies But it is also useful to describe what happens in a crystal considering diagrams that are in Real space.