

# PH 61013 - Principles of Quantum Devices :-

Lecture - 1

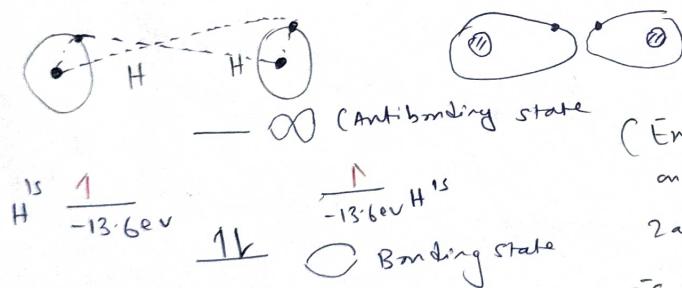
- This course is about the changes induced in the properties of devices (such as diodes), when they are diminished to smaller sizes. (i.e. to the level of atoms).
- We will consider both Electrical & Optical properties of the devices.

Evaluation:-

- ↳ End Sem - 50
  - ↳ mid Sem - 30
  - ↳ Project - 20
- Report (10)      viva (10)

Pre-req's :-  
 → quantum mechanics  
 → solid state physics

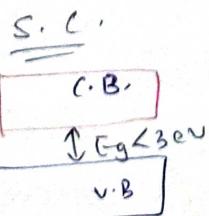
H<sub>2</sub> formation



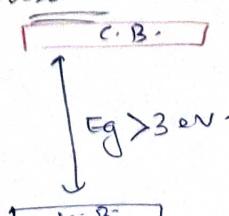
(Energy always minimizes, and hence when H<sub>2</sub> atom is formed, 2 atoms come close to each other, hence it's experience diff. force, hence the atomic orbitals splits (molecular orbital theory))

In crystals such as Si etc. (N) no. of such e's together form the structure. (so  $= 2N$  no. of states would be created). As N is v. large, we can consider the discrete levels to be a continuum. (Hence bonds are formed in S.C.)

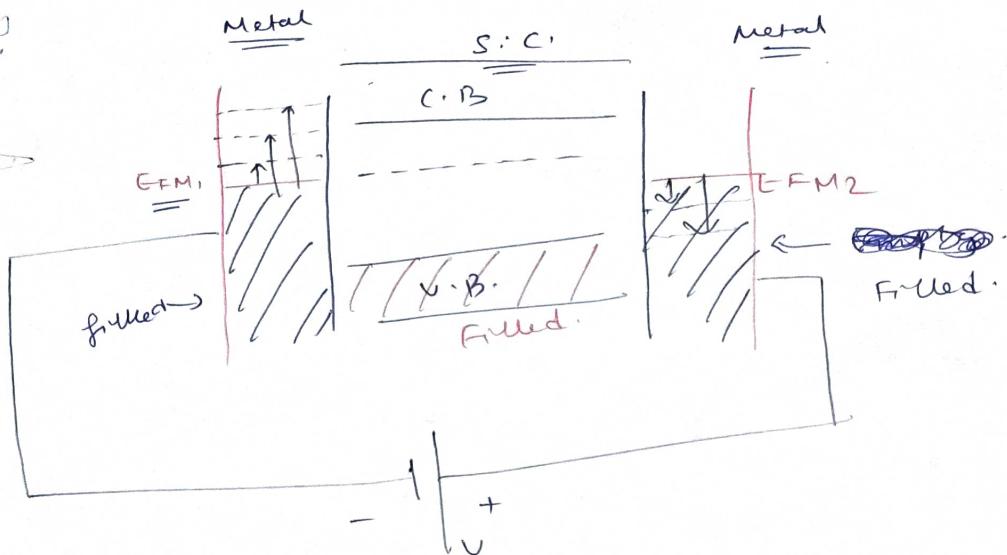
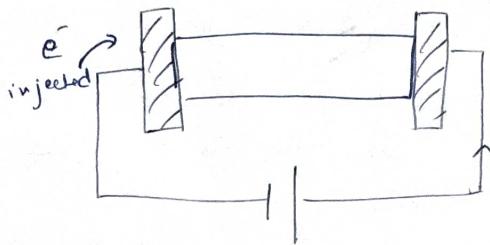
Metal



Insulator



Now, let's analyze the V-I curve of a Semicondutor at  $T = 0\text{ K}$ .



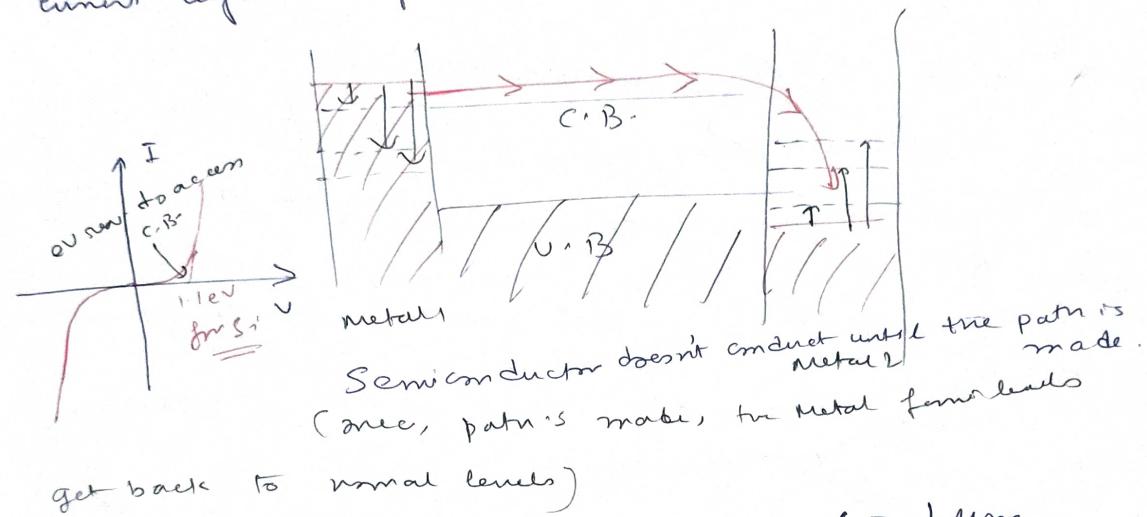
When  $V$  volts are applied, the energy of the  $e^-$  which enters into the metal is  $eV$ .

The injected  $e^-$  of energy  $eV$ , moves into the metal and occupies a state above the Fermi level. The  $e^-$  stays there as it cannot move to the S.C. as no valid empty state is available at the energy the  $e^-$  was pumped into with.

To maintain conservation of charge, the free metal contact loses an  $e^-$  from a filled state below the Fermi level. Hence the Fermi level moves towards.

(Now voltage is increased, and some more  $e^-$ s are pumped to higher energy states.)

This process continues, as the Fermi level of one metal contact goes up, the other will go down; as long as the  $E_{FM,1}$  (Fermi level of metal contact 1) does not come to a comparable energy level as the C.B. edge of the S-C. Once this happens, a channel through the semiconductor is formed, and current begins to flow.



# In normal microelectronics, dimension  $L = 1 \text{ nm}$   
 $(400-500 \text{ atoms})$

For  $L = 1 \text{ nm}$  (3 to 4 atoms) would be true,  
 (so classical methods won't work, and we need separate  
 physics to analyze these devices)  
 This is what we will do in this course. (Special physical  
 phenomena)

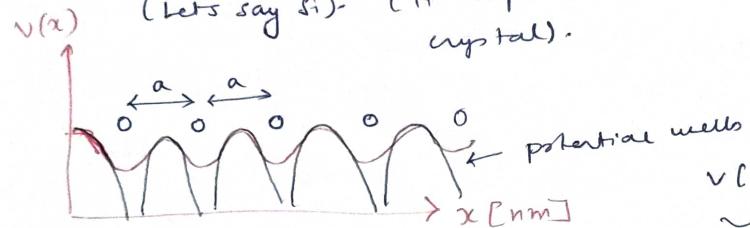
# Principles of Quantum Devices

class 2

The dispersion relation ( $E$  vs  $k$ ) and the density of states relations can be derived from the "Kronig - Penney Model".

→ In reality we have 3D arrangement

→ It is a simplified model assuming 1D arrangement of atoms  
 (lets say si) - (it explains the behavior of e<sup>-</sup>s in periodic lattice crystal).  
 (Read more on internet)



$$v(x) = \sum_{i=1}^{\infty} v_i(x)$$

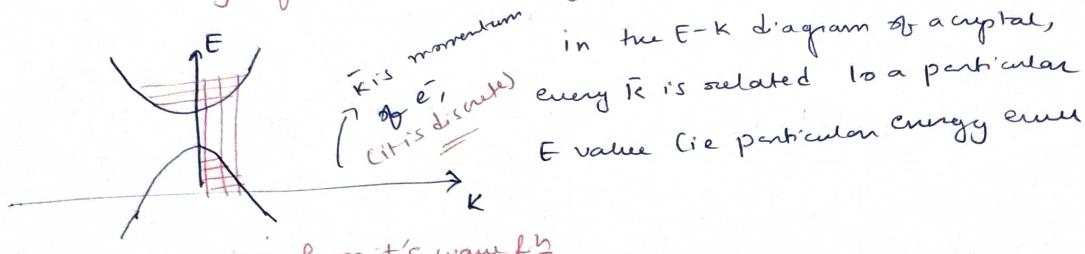
→ overall potential profile.

(For simplification of calculation, we can assume the well structure as a sine wave).

if we solve the Schrödinger eqn. given the constraints of the Kronig Penney model, and solve for  $E$  :-

$H\psi = E\psi$ , then from the soln. of  $E$ , we can find the Energy band diagrams of a crystal.

The solution for  $E$  is done computationally using a technique called.  
 DFT → Density functional theory.



The  $k$  value comes from its wave f<sup>n</sup>

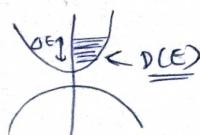
What is Density of states?

Density of states  $D(E)$ , tells us the no. of energy states we have per unit energy ( $\Delta E$ ) per unit volume

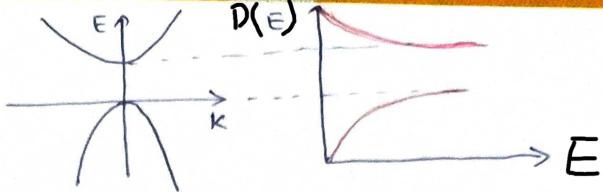
i.e., no. of energy states in  $\Delta E$

we can find the 'E vs  $D(E)$ ' curve from the E-K curve as:-

$$D(E) \propto \frac{1}{(\Delta E/dk)}$$



$$\text{As } D(E) \propto \frac{1}{\frac{d(E)}{dk}}$$

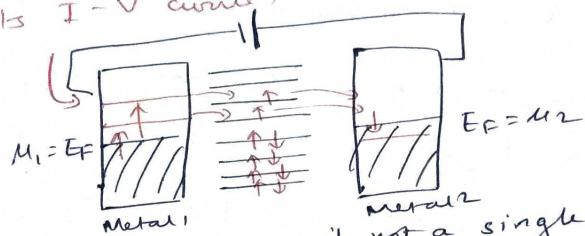
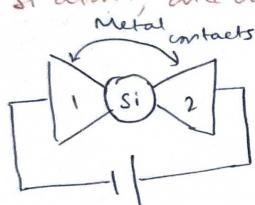


# if slope is less in  $E - k$

curve, that means more states are present  $\Rightarrow D(E)$  is more.

# if slope is more, less states are counted  $\Rightarrow D(E)$  is less.

Now, let us think of an interesting problem. Just as we had studied the flow of current through a bulk Si Semiconductor, let us analyze what happens when voltage is applied across a single Si atom, and analyze its I-V curve.



we can also think of it as a nano particle, if not a single atom. By nanoparticle we mean that the no. of atoms is so less that the Energy levels are still discrete.  $\Rightarrow$  Bands are not formed.

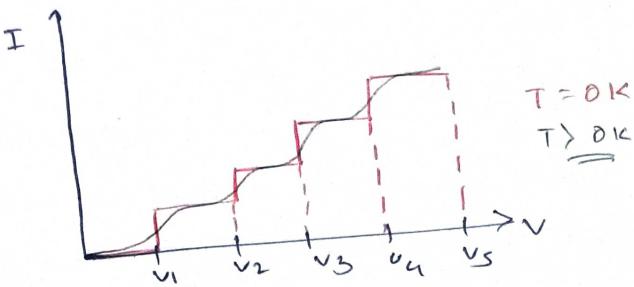
) In this scenario some of the energy states (bottom energy levels) are completely filled, while upper energy levels are completely empty.

) When voltage is applied, some electrons are pumped in Metal 1, and fermi level ( $E_F$ ) is made to go up, and some  $e^-$  is removed from metal 2, hence fermi level ( $E_F$ ) is made to go down.

) No current flows until  $E_F$  goes above an empty energy levels when it does a channel is formed and current flows.

(The current however does not continuously increase, as as energy level can only take  $2e^-$  at most). So current remains constant.

) When voltage is then increased such that another energy level goes beneath  $E_F$ , only then the current increases to another level and stays steady there (So the current increases step by step).

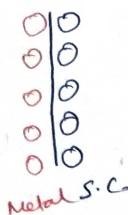


An possibility of tunnelling:-

→ The junction also has its own potential barrier the  $e^-$  needs to tunnel through from the metal to the S.C. particle →  $e^-$  does not (in general) have any extra energy, but if the metal - S.C. contact is v. clean, then there is some finite probability of ~~no~~ tunnelling.

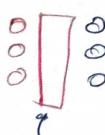
To get a v. clean junction, (Molecular Beam Epitaxy) MBE is utilized.

in MBE, interface is grown atom by atom, in ultra-high vacuum ( $10^{-10} - 10^{-11}$  m. bar).

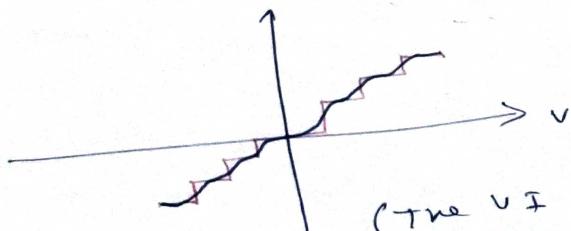


This process is v. costly.

If the junction isn't clean, we can get formation of an unwanted material in the junction, rendering the device useless.



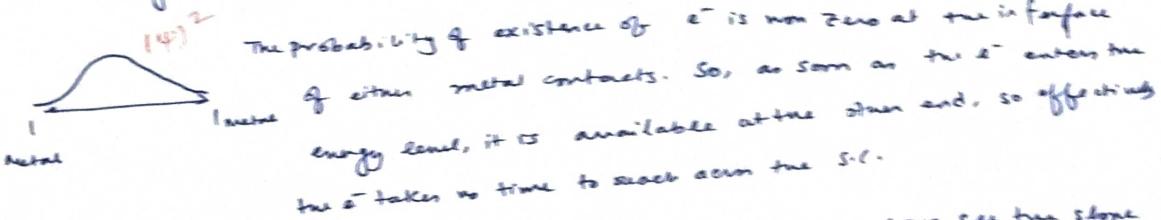
( $Au_x Si_{1-x}$ )



(The V-I curve is called Coulomb blockade & staircase)

Now, where is the  $e^-$  located and how fast it travels across the energy level :-

According to probability density  $f_{\text{m}}^{\infty}$  of an electron in the energy level,



Now, if we ~~try~~ see the I-V curve of the device, we can see the slope is 0 at some places &  $\infty$  at other places, so effectively, its resistance varies b/w 0 &  $\infty$ . Thus R can't be defined for such systems.

Hence, the concept of Quantum Conductance was introduced.

$\Rightarrow$  In the definition of current  $I = \frac{q}{T}$ , T has no meaning in this case as Time taken for  $e^-$  to travel across energy level is 0.

$\Rightarrow$  However, the time introduced in this case is the time taken for the energy to cross the contact & Energy barrier (@ the metal-S-I.  $j =$ )

$$\therefore I = \frac{q}{t} \quad \text{Time is in order of picoseconds.}$$

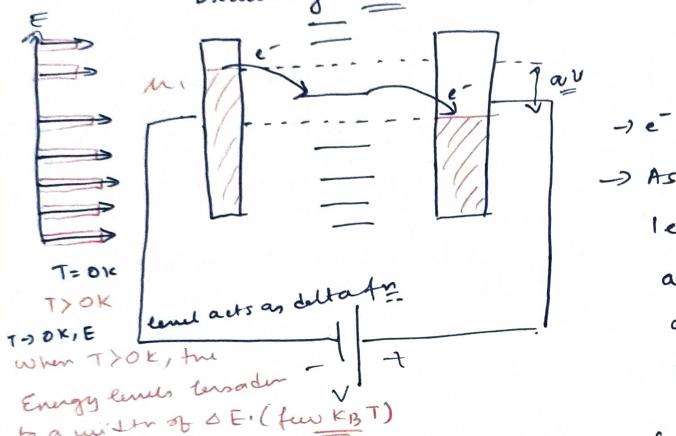
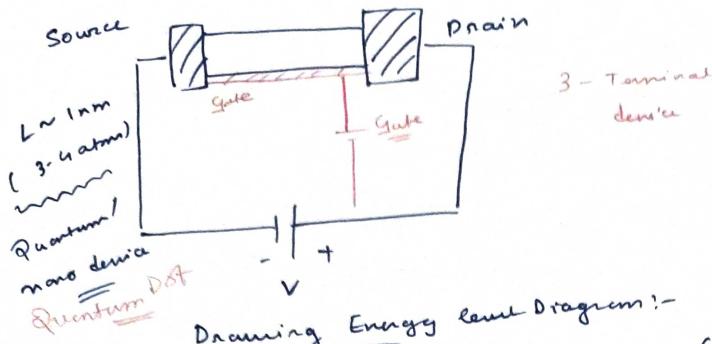
Parameter which effectively acts as Energy  $\gamma = \frac{q}{t}$   $\gamma = Js$

Hence, we define a parameter  $\frac{\gamma}{t}$ , where  $\frac{\gamma}{t}$  is the rate of charge transfer unit [ $\text{Vs}^{-1}$ ]

$$\gamma_1 = \gamma_2 = \frac{\gamma}{t} \quad (\text{if both metal contacts are identical}).$$

$\therefore$  For both contacts total time:-

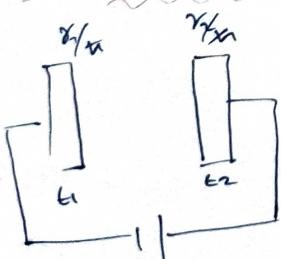
$$\therefore t_{\text{ps}} = \frac{t}{\gamma} \quad t_{\text{tot}} = \frac{2t}{\gamma}.$$



Now if the voltage is not increased further, then only  $e^-$  stays in the Energy level. (As it stays in the S.C.), The one electrons addition makes the nano. S.C. charged. (This is called charging of quantum Dot; this is called charging effect).

Q. What is the effect of charging on Q. Dot? → Think in our

Assuming



$$I = \frac{a}{t_1 + t_2}$$

$$\Rightarrow I = \frac{a \cdot 2\pi r}{\frac{\pi r}{d} + \frac{\pi r}{d}} = \frac{a \cdot 2\pi r}{2\pi r} \quad \left\{ \frac{a}{\frac{\pi r}{d}} = \frac{a}{2\pi r} \right\}$$

Value of  $\gamma$  comes from the design

of the device. [how clean the junction is]

$$E = \sum_{i=1}^n V_i \Delta n(x)$$

$$V = \sum_{i=1}^n V_i S_i(x)$$

$$I = \frac{a \gamma}{2\pi}$$

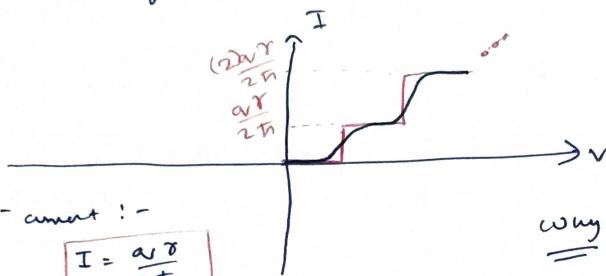
Expression  
of current  
from 1 e

Now using the values  
if we calculate  
 $I = E \Psi$

we will get diff. energy levels for Au, Si &  $\text{Au}_{1-x}\text{Si}_{x}$ .

∴ the  $\gamma$  for pure Au-Si interface will be different from the b/w  
 $\text{Au}-(\text{Au}_{1-x}\text{Si}_x)\text{-Si}$ .  
in both the cases.

∴  $\gamma$  for Au-Si will be more than the  $\gamma$  for  $\text{Au}-(\text{Au}_{1-x}\text{Si}_{x})-\text{Si}$ .  
(So, better the interface, higher the  $\gamma$ , better the current flow).



$T = 0K$  }  
 $T > 0K$  }  
when  $T > 0K$ , the  
Energy levels widen  
to a few  $k_B T$ .

(e<sup>-</sup> current :-

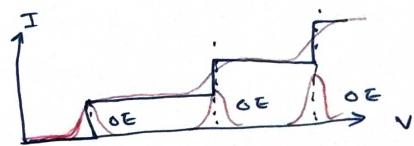
$$I = \frac{ar}{2t}$$

why? in Schrödinger Eqn.

$$(H\Psi) = E\Psi$$

When temp. increases, the atoms vibrate,  
and moves somewhat, therefore, its  
potential position varies slightly; so the sum of  
position varies slightly; so the sum of  $E$  widens.  
 $E$  also varies as  $V$  varies. So, the sum of  $E$  widens.

The widening can be approximated as a Gaussian dist. assuming  
The vibration is in a gaussian way.  
(The broadening of  $E$ -level increases  
with temp.).



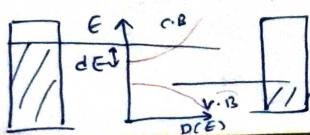
$$\approx V = f E \cdot dE$$

$$V = \int E \cdot dE$$

gaussian.  $f \approx$

$$V \rightarrow \text{Error of } f \approx \text{few}$$

The current is simply not the no. of e<sup>-</sup> injected by the battery, it depends on the  
 $D(E)$  available for taking up the e<sup>-</sup>.



Current depends on the D.O.S. available  
in the diff. b/w.  $m_1$  &  $m_2$ .  $\leftarrow$  no. of states.

$$\therefore I_{\text{total}} = \frac{ar}{2t} \int_{m_1}^{m_2} D(E) dE$$

# Principles of Quantum Devices:-

Class 4

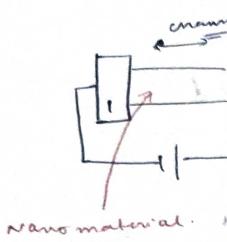
$$D(E), \text{ general form} :- D(E) \propto E^{N/2 - 1}$$

$N \rightarrow \text{dimension}$

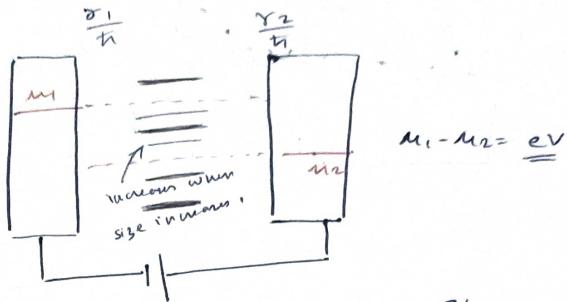
$$\underline{N=3} \quad D(E) \propto E^{1/2}$$

$$\underline{N=2} \quad D(E) \text{ independent of } E$$

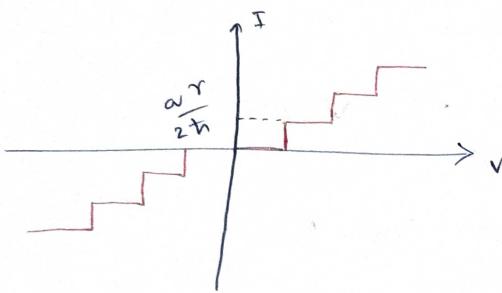
$$\underline{N=1} \quad D(E) \propto E^{-1/2}$$



- nano material
- Quantum Dot
- 2D material
- 1D material



$$m_1 - m_2 = \underline{\underline{eV}}$$



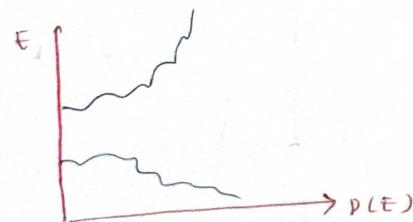
$$I e^- \text{ current} :- \quad I = \frac{\alpha}{t_1 + t_2}$$

$$\Rightarrow I = \frac{\alpha}{\frac{n}{d_1} + \frac{n}{d_2}}$$

$$(\text{if } d_1 = d_2)$$

$$\Rightarrow I = \frac{\alpha r}{2n}$$

When the channel size increases, the energy levels keep coming closer to one another, until we get a bulk material and then we see the formation of bands (as the levels overlap after coming v. close).



∴ In such cases, total current is :-

$$I_{\text{total}} = \frac{\alpha r}{2n} \int_{m_1}^{m_2} D(E) \cdot dE$$

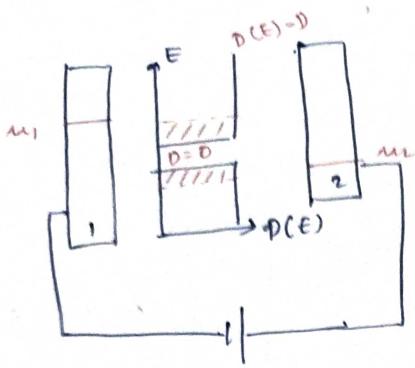
$$I \rightarrow \text{for } 1 e^-$$

No. of  $e^-$   
which take  
part ( $i.e.$ )  
no. of states b/w  
 $m_1, m_2$ ).

Here, we have assumed  $r$  is not a function of Energy.

(However, in reality it is a  $f(E)$ , we will consider this later.)

Let us consider a simplified case where  $D(E)$  is independent of  $E$  :-



$$D(E) = D$$

$$(M_1 - M_2 = \alpha v)$$

$$I = \frac{\alpha v}{2\pi} \int_{M_2}^{M_1} D(E) dE$$

$$I = \frac{\alpha v}{2\pi} \cdot D \int_{M_2}^{M_1} dE = \frac{\alpha v}{2\pi} D (\text{term})$$

$$I = \frac{\alpha v}{2\pi} D \cdot \alpha v V$$

$$I = \frac{\alpha^2 D \cdot 2\pi}{2\pi h} \alpha v$$

$$\Rightarrow I = \frac{\alpha^2 v}{h} (\propto D \alpha)$$

$$\Rightarrow g = \frac{I}{V} = \frac{\alpha^2}{h} (\propto D \alpha)$$

Later we will see, this is an integral number.

So, Conductance is quantized.

The quantum of conductance is :-

$$\left( \frac{\alpha^2}{h} \right)$$

This is a constant.

How calculate the value of this constant?

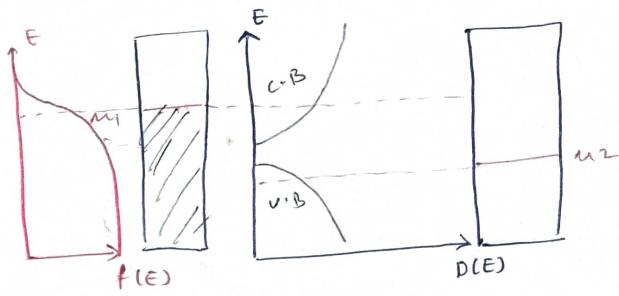


$$\frac{dI}{dV}$$

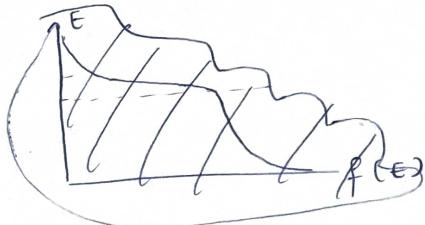


$$T=0$$

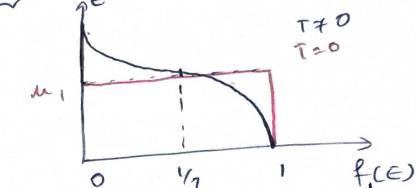
$$T > 0$$



$T \neq 0$

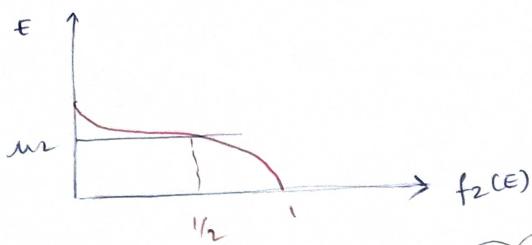


For contact 1



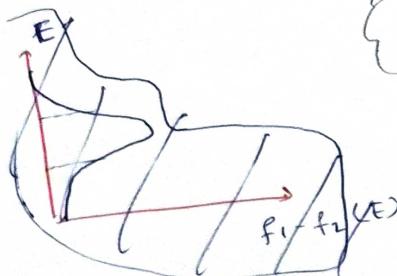
$$f_i(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$

For contact 2



$D_i(E)$  decides if states are present  
not

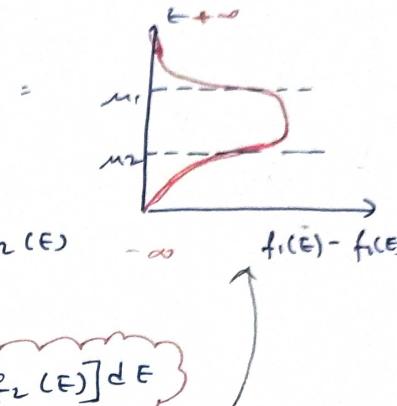
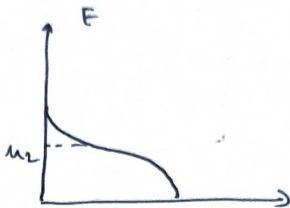
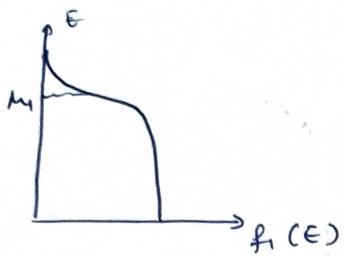
$f_i(E)$  decides if states are filled  
or not,



$$I = \frac{\alpha v}{2\pi} \int_{-\infty}^{\infty} (f_1(E) - f_2(E)) \cdot D(E) dE$$

As non zero probabilities of  $e^-$  presence  
above  $\mu_1$   
& non-zero probability of  $e^-$  below  $\mu_2$

How will  $f_1(E) - f_2(E)$  look like?



So,

$$I = \frac{av}{2\pi} \int_{-\infty}^{\infty} \sigma D(E) [f_1(E) - f_2(E)] dE$$

Confined around  $\underline{\mu_1 - \mu_2}$

rest goes to 0 almost.

Let us see if the expression

$$I = \frac{\alpha \gamma}{2\pi} \int_{-\infty}^{\infty} D(E) [f_1(E) - f_2(E)] dE \quad \text{--- (1)}$$

conforms with Ohm's law.

For bulk material :-

$$\Rightarrow \text{conductivity} : G = G \cdot \frac{A}{L} \cdot \left( A \rightarrow \text{area of channel} \right) \quad \left( L \rightarrow \text{length of channel} \right)$$

Conductance

conductivity

From Eqn. (1), we have to show

$$(G \propto A) \quad \& \quad (G \propto \frac{1}{L})$$

From Eqn. (1) we have got :-

$$I = \frac{\alpha \gamma}{2\pi} \int_{-\infty}^{\infty} D(E) \{ f_1(E) - f_2(E) \} dE = \frac{\alpha^2}{\pi} (D \propto \gamma)^{\vee}$$

$$G = \frac{I}{V} = \frac{\alpha^2}{\pi} (D \propto \gamma)$$

The only term related  
to  $A \& L$  is  $D$ .

We know,  $D \propto \text{volume} \therefore D \propto A, D \propto L$

$$\therefore G = \frac{\alpha^2}{\pi} \propto \gamma (A \cdot L)$$

What's going wrong?  $\Rightarrow \gamma$

$(\frac{\gamma}{h})$  depends on velocity and channel length  $\therefore \frac{\gamma}{h} \propto \text{expression of rate. (Vs)}$

$$G \propto A$$

$G \propto L \leftarrow \text{incorrect as } G \text{ should be} \propto \frac{1}{L}$

$$\frac{\gamma}{h} = \frac{v}{L}$$

$v$  is velocity

Now, putting this we get:-

$$G = \frac{a^2}{h} \pi \times A L = a^2 \pi (A h) \cdot \left(\frac{V}{h}\right) = a^2 \pi (Av)$$

Now, this is also invalid, as now  $G$  is independent of  $(L)$ .

Now, if we look some more, we find; the velocity of  $e^-$ ,  $v$  is related as:-

$$v = \frac{2D}{L}$$

( $D \rightarrow$  Diffusion constant).

$$\frac{D}{h} = \frac{2D}{L^2}$$

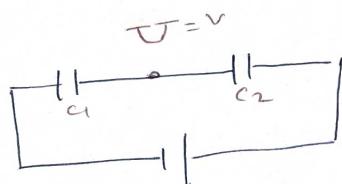
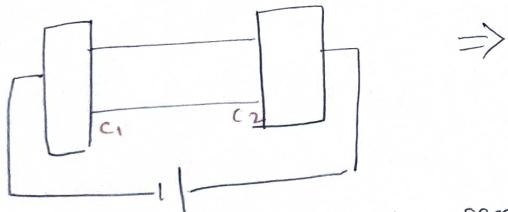
So,  $G = 2a^2 \pi A \cdot \frac{D}{L} = 2a^2 \pi D \left(\frac{A}{L}\right)$

$$\therefore G \propto A$$

$$G \propto \frac{1}{L}$$

(So, now we can see, this relation conforms with Ohm's Law!) and the eqn (1) holds good.

Another parameter which needs consideration is channel potential ( $V$ ). This channel potential comes due to junction capacitance.

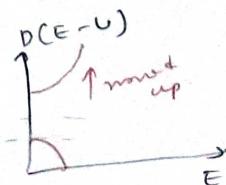
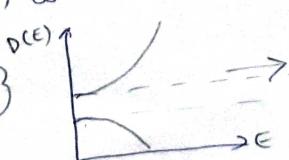


When  $e^-$  is injected into the semiconductor, the junction capacitance gets charged, and hence the channel potential increases. When  $e^-$  is taken out of the channel, the capacitor gets discharged, and hence channel potential decreases. (D.O.S. remains unchanged)

How will this affect the current?

This channel potential  $V$ , moves the DOS curve up when it's charged, and comes down to default level, when discharged.

$$I = \frac{a\pi}{h} \int_{-\infty}^{\infty} D(E-U) [f_1(E) - f_2(E)] dE$$



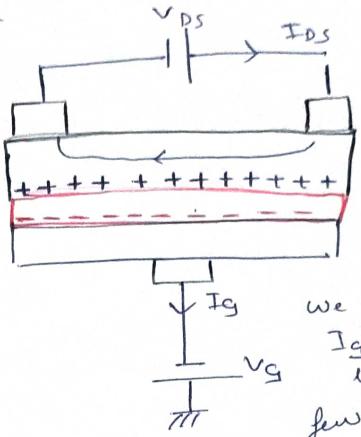
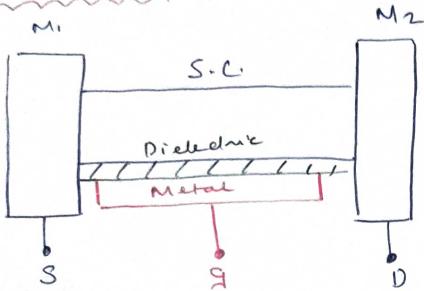
$V_{ds}$  has 2 components :-

$$U = U_L + [ \text{Diagram of a capacitor symbol with arrows indicating potential difference} ]$$

Some other terms will be discussed  
(due to the capacitor) in next class.

Laplace potential

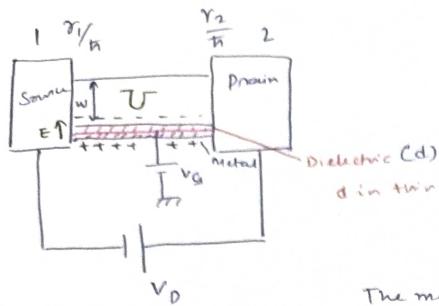
Let us discuss 3 terminal devices a bit :-



We want  
 $I_g$  to  
be

few  
orders of  
mag ≈ less  
than  ~~$I_{ds}$~~   $I_{ds}$

(ideally 0)



$$I = \frac{e}{2\pi} \int dE D(E-U) [f_1(E) - f_2(E)]$$

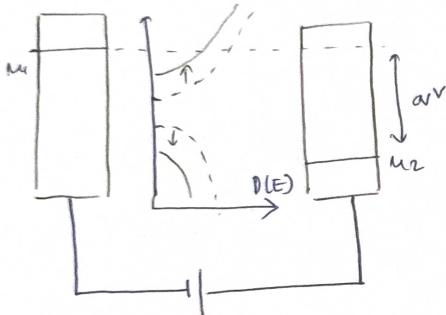
d in thin film transistor  
d ≈ 100nm

(1)

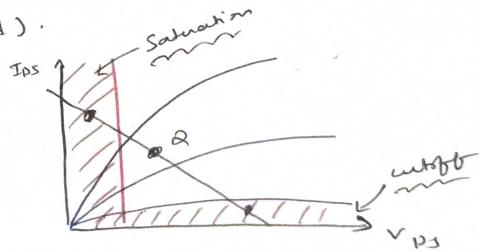
The mag. of E field induced in the dielectric layer is:-

$\int D(E) \text{ in channel}$

$$E = \frac{V_G}{d} \quad (\text{As dis } v \text{ small, the E field would be } v \cdot \text{high})$$



⇒ The  $D(E)$  levels might shift up/down depending on the  $V$  value, so the current flowing through the channel might go up/down due to charging of the channel. (if this current change is v. significant, the operation pt., & pt. of the transistor might go from cutoff to saturation, which is not at all wanted).



The gate layer should always be thinner than channel length:-

(Different designs of gate are done, so

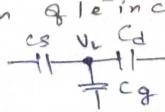
that  $V$  doesn't change by much.

Now → default no. of  $e^-$  in channel when  $V_G = 0$

$V \rightarrow$  total potential of channel.

$$V = V_L + V_0 (N - N_{0v}) \quad (2)$$

↳ potential for addition of  $1e^-$  in channel



$$\text{Eg: } L = 100 \text{ nm}$$

$d = 10 \text{ nm}$

↳ can't go any smaller as it will cause leakage & current, so  $I_D \uparrow$ .

Now,  $N$  is the no. of  $e^-$ s stored in the channel ( $N_{\text{ear}} \rightarrow$  is  $\infty$ , i.e. no. of  $e^-$ s in the channel), we can find  $N$  as:-

$$N = \int dE n(E) = \int dE D(E) f(E)$$

$\hookrightarrow$  fermi function for channel.

$D(E)$  &  $f(E)$  are not known for nano devices (e.g. Q. wire, Q. dot etc.)

$$N = \int dE D(E) \left[ \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} \right]$$

$\hookrightarrow$  fermi  $f_m^{\pm}$  for why?  
channel.

$f_1 \rightarrow$  fermi  $f_m^{\pm}$  for contact 1  
 $f_2 \rightarrow$  fermi  $f_m^{\pm}$  for contact 2

$\rightarrow$  probability of occupancy :- depends on contacts

$(f_1, f_2)$  &  
rate of transfer ( $\gamma_1, \gamma_2$ )

$$\therefore I = \frac{eV}{h} \int dE D(E - U) \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} [f_1(E) - f_2(E)] \quad (1)$$

$(1), (2), (3)$  are self consistent coupled eqns.

# Principles of Quantum Devices

class - 7

Equations from last class:-

$$I = \frac{a}{\pi} \int dE D(E-U) \left[ \frac{\tau_1 \tau_2}{\tau_1 + \tau_2} \right] (f_1(E) - f_2(E)) \quad (1)$$

$$U = U_L + U_0 (N - N_{0av}) \quad (2)$$

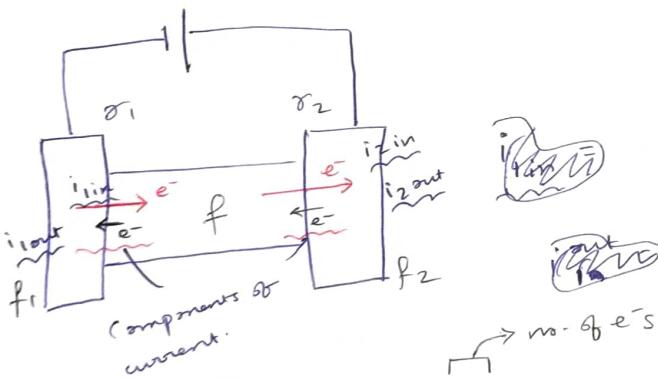
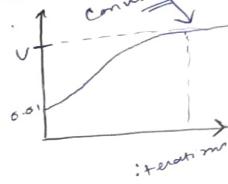
$$N = \int dE n(E) = \int dE D(E-U) \left[ \frac{\tau_1 f_1 + \tau_2 f_2}{\tau_1 + \tau_2} \right] \quad (3)$$

from fr. q. m. current

(1), (2), (3) are coupled equations.

Solution is done numerically, i.e. we start off with an assumption of value (lets say  $U=0.01$ , use this to find  $N$ , use  $N$  to find  $U$  and so on till the values stabilize). The values will eventually converge to a value.

Once the value of  $U$  converges, we can use that in eqn (1).



$$i_1^{\text{out}} = \frac{a \tau_1}{\pi} \int_{-\infty}^{\infty} dE D(E-U) [f] \quad \begin{matrix} \text{Density of states} \\ \text{rate} \end{matrix}$$

can be ignored as controlled by  $V_{0av}$

$$i_1^{\text{out}} = a \cdot \frac{\tau_1}{\pi} \int_{-\infty}^{\infty} dE D(E) [f]$$

$a$   $\tau_1$   $n$   $f$  from S.C. to contact

if  $f_1 = f \rightarrow$   
no current, as  
fermi function diff.  
must be true for  
 $e^-$  to flow.

$$i_1^{in} = \alpha \frac{\tau_1}{\hbar} \int_{-\infty}^{\infty} dE D(E) [f_1]$$

from contact to S.C.

$$\therefore i_1 = i_1^{in} - i_1^{out}$$

$$i_1 = \alpha \frac{\tau_1}{\hbar} \int_{-\infty}^{\infty} dE D(E) [f_1 - f]$$

Similarly

$$i_2 = (i_2^{in} - i_2^{out}) = i_2^{out} - i_2^{in} = \alpha \frac{\tau_2}{\hbar} \int_{-\infty}^{\infty} dE D(E) [f - f_2]$$

Consistency of direction.

$$\text{At equilibrium } \therefore i_1 = i_2 = I$$

$$\therefore \frac{\alpha \tau_1}{\hbar} \int dE D(E) [f_1 - f] = \frac{\alpha \tau_2}{\hbar} \int dE D(E) [f - f_2]$$

$$\Rightarrow \tau_1 [f_1 - f] = \tau_2 [f - f_2]$$

$$\Rightarrow \tau_1 f_1 - \tau_1 f = \tau_2 f - \tau_2 f_2$$

$$\Rightarrow (\tau_1 + \tau_2) f = \tau_1 f_1 + \tau_2 f_2$$

$$\Rightarrow f = \frac{\tau_1 f_1 + \tau_2 f_2}{\tau_1 + \tau_2}$$

Put the value of  $f$  in either  $i_1$  or  $i_2$ ,

$$\therefore I = \frac{\alpha \tau_2}{h} \int dE D(E) \left[ \frac{\tau_1 f_1 + \tau_2 f_2}{\tau_1 + \tau_2} - f_2 \right]$$

$$\Rightarrow I = \frac{\alpha \tau_2}{h} \int dE D(E) \left[ \frac{\tau_1 f_1 - \tau_1 f_2}{\tau_1 + \tau_2} \right] \quad \text{Take } \frac{\tau_1}{\tau_1 + \tau_2} =$$

$$\Rightarrow I = \frac{\alpha}{h} \int dE D(E) \frac{\tau_1 \tau_2}{\tau_1 + \tau_2} [f_1 - f_2]$$

Syllabus

- I. Nano & Quantum Device - Theoretical Development / Understanding of Charge Transport. (20s)
- II. Calculation of Density of states of different Quantum systems:- (30marks)
- Graphene
  - Carbon Nano Tubes } 10 & 20 System. (midsem) (30marks)
- III Superconducting Quantum Devices (End sem) (50 marks) (30s)
- Q bit (Superconducting, JJ)
- IV Current status of Quantum Technology.

— x —

Principles of Quantum Devices:-

$$I = \frac{a^2}{h} \int dE D(E-U) \left[ \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \right] (f_1(E) - f_2(E))$$

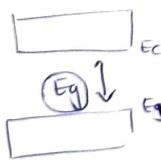
$$N = \int dE D(E-U) \left[ \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} \right]$$

$$V = V_L + V_0 (N - N_{av})$$

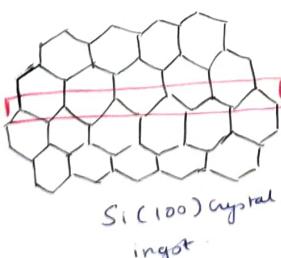
These eqns. valid for any kind of Device (Nano or Bulk)  
Coupled eqns.  
Solved using computational methods.  
— x —

→ For solving any of these equations, knowing the Density of States is important.  
we can find the Density of states by using DFT (Density Functional Theory)  
or Experimentally

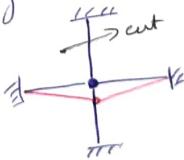
How do we measure the Bond gap of a Semiconductor?



Laser cut



(Surface rearrangement happens)  
leaves dangling Si bonds.

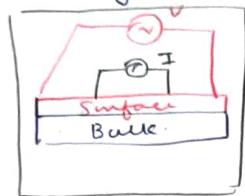


(Rearranging of the Si on the surface takes place to go to its equilibrium position)

(So, the Si wafer surface and the bulk have different crystal structures, and hence the solution of  $H\psi = E\psi$  on surface & bulk is different)

Different bond structures in surface & bulk.

If we try to find the band gap using surface probing :-

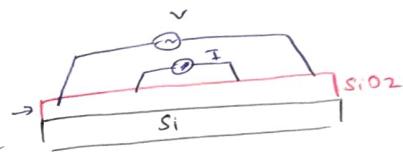


UHV

(UHV)  $10^{-10}$  to  $10^{-11}$  mbar

Then even in Ultra high vacuum the correct band structure cannot be measured as surface and bulk bands are different.

# If we try to probe the Si wafer in normal condition, then an oxide layer ( $\text{SiO}_2$ ) is formed automatically on its surface. So surface probing using Electrical parameters again fail.

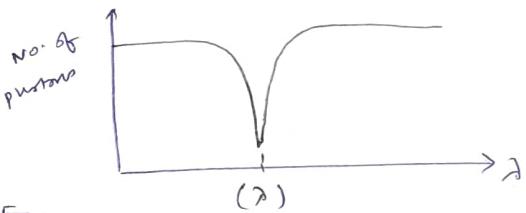
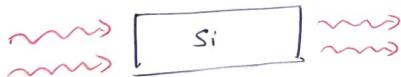


$\text{SiO}_2$   
affecting  
measured  
current

→ Technically we are only measuring leakage current through oxide.

(Optical)

In actuality, Eg measurement of Si is done through Absorption study



$\lambda$  is absorbed photon corresponding to Eg.

$$\text{so } Eg = \left( \frac{hc}{\lambda} \right).$$

↑ This is how  
Bandgap is calculated.

(Si don't emit photons, so  
emitted photon is not  
considered.)

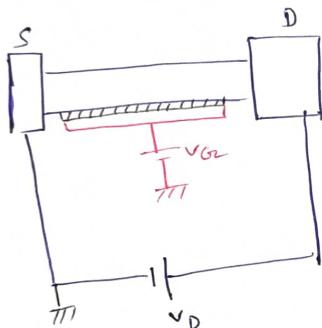
(class - 9)

$$I_D = \frac{\alpha}{h} \int dE D(E-U) \left\{ \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \right\} [f_1(E) - f_2(E)] - C_1 \quad (1)$$

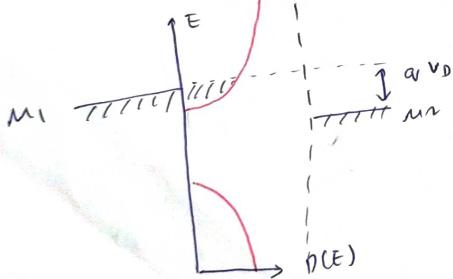
$$V = V_L + V_0 (N - N_{\text{ear}}) \quad (2)$$

$$N = \int dE D(E-V) \left[ \frac{f_1 \gamma_1 + f_2 \gamma_2}{\gamma_1 + \gamma_2} \right] - C_2 \quad (3)$$

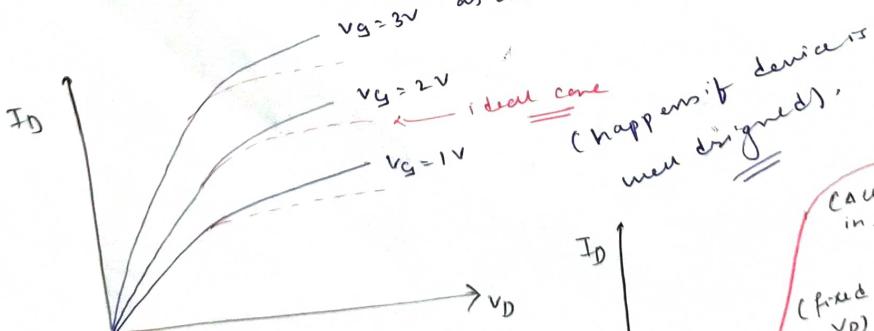
Characteristic coupled equations explaining the functioning of the device.



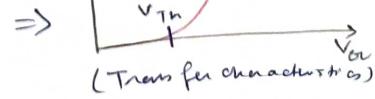
Now, we will try to qualitatively analyze the ear<sup>m</sup> and find the I-V relation of the device.



$V_{Gn}$  is responsible for  $D(E)$  shift up/down in  $E$ .  
 As  $V_G \uparrow$ ,  $D(E)$  moves down, and therefore more  $D(E)$  lies in reverse ( $\mu_1 - \mu_2$ ). So current  $I_D$  increases as channel width increases.



(As  $V_G \uparrow$ ,  $D(E) \uparrow$ ,  $I_D \uparrow$ )



if  $f_1(E) \approx f_2(E)$  (very close) i.e.  $V_D \rightarrow V$ -small (current due to small voltage  $V_D$ )

$\hookrightarrow$  we study in low voltage because in general, battery (small size) produce low voltage

$$f_1(E) = f_2(E) = f \cdot \text{surface current}$$

$$\therefore N = \int dE D(E-U) \left\{ \frac{\gamma_1 f + \gamma_2 f}{\gamma_1 + \gamma_2} \right\} \Rightarrow \int dE D(E-U) f(E) \quad (1)$$

No. of carriers in channel.

if  $V_D \rightarrow$  very high (wide window) - (i.e., wide channel).

$$f_1(E) \gg f_2(E) \therefore f_1(E) - f_2(E) \approx f_1(E) \cdot$$

Current is driven by first contact.

In such case:-

$$i_1 = \frac{\alpha}{n} \int dE D(E-U)$$

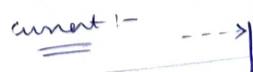
$$i_2 = \frac{\alpha}{n} \int dE D(E-U)$$

$$(i_1 = i_2 = I)$$

$$\therefore I = \frac{\alpha}{n} \int dE D(E-U) f_1(E) \quad (\text{Assume } \gamma_1 = \gamma_2 = \gamma \text{ for simplification})$$

$$\therefore I = \boxed{\frac{\alpha \gamma N}{L}} \quad \leftarrow \text{At v. high } V_D, I_D \text{ is not any more}$$

fn. of  $V_D$

current :- 

$$\therefore \frac{\alpha N}{L} V = \frac{\alpha \gamma}{n} \frac{N}{L} N$$

$$\Rightarrow \boxed{\frac{\gamma}{n} = \frac{V}{L}}$$

$\frac{N}{L} \rightarrow e^- \text{ density / length}$

$$\therefore I = \frac{\alpha \frac{N}{L} \times V \times t}{L} = \alpha \frac{N}{L} V$$

$$I_D = \frac{a}{h} \int dE D(E-U) \left[ \frac{\sigma_1 \sigma_2}{\sigma_1 + \sigma_2} \right] [f_1(E) - f_2(E)] - c_1$$

$$N = \int dE D(E-U) \left[ \frac{\sigma_1 f_1 + \sigma_2 f_2}{\sigma_1 + \sigma_2} \right] - c_2$$

$$V = V_L + V_0 (N - N_{eq}) - c_3$$



From last class :-

$$\frac{\sigma}{h} = \frac{v}{L}$$

$\left. \begin{array}{l} \text{Big conductor} \\ \text{CD. if fused scattering} \\ \Delta \rightarrow \text{mean free path} \\ L \rightarrow \text{length of conductor} \end{array} \right\}$

$$! (L \gg \Delta) \Rightarrow \frac{\sigma}{h} = \frac{v}{L} \left( \frac{\Delta}{\Delta + L} \right)$$

$$\Rightarrow \frac{\sigma}{h} = \frac{v}{L} \cdot \frac{\Delta}{L}$$

$$\left. \begin{array}{l} \text{Small conductor} : (L \ll \Delta) \Rightarrow \frac{\sigma}{h} = \frac{v}{L} \\ (v \cdot \text{short channel}) \end{array} \right\} \text{Ballistic transport}$$

We can also describe the above by mean collision time ( $\tau_{sc}$ ).

$$\Delta = v \cdot \tau_{sc}$$

$$\text{No of collisions} : n = \frac{T_{transit}}{\tau_{sc}}$$

$(T_{transit}) \rightarrow$  time taken to go across the channel.

$$\therefore \text{Total length} \Rightarrow L^2 = \frac{T_{transit}}{\tau_{sc}} (\Delta)^2 = \frac{T}{\tau_{sc}} (v \cdot \tau_{sc})^2 \quad \left( \begin{array}{l} \text{Squared because } \Delta \\ \text{is mean squared distance} \end{array} \right)$$

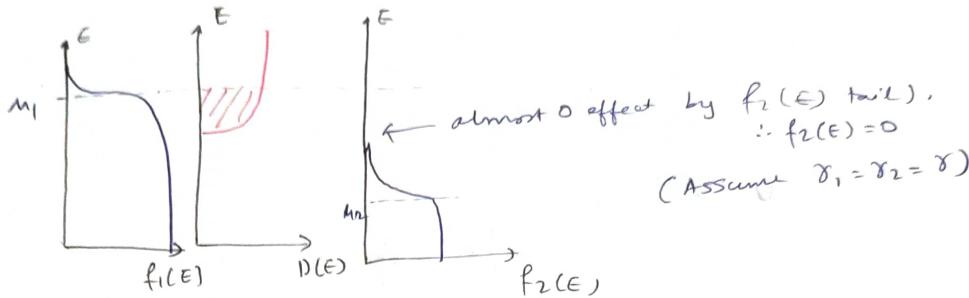
$$\Rightarrow \frac{1}{T} = \frac{1}{L^2} v^2 \tau_{sc}$$

$$\Rightarrow \frac{1}{T} = \frac{v \cdot (v \tau_{sc})}{L^2} = \frac{v}{L} \cdot \frac{\Delta}{L}$$

$$\Rightarrow \frac{\sigma}{h} = \frac{1}{T} = \frac{v}{L} \cdot \left( \frac{\Delta}{L} \right)$$

$$\Rightarrow \frac{\sigma}{h} = \frac{v}{L} \left( \frac{\Delta}{L} \right) \quad \leftarrow \text{Expression for Diffusive Transport}$$

Finding ON current ( $I_{ON}$ ), for high  $V_D$ : (Wide  $\mu_1 - \mu_2$  window)



$$I_{ON} = \frac{eV}{h} \int dE D(E-U) \frac{\gamma}{2} f_1(E)$$

$$N = \int dE D(E-U) \frac{f_1(E)}{2}$$

$$\therefore I_{ON} = \frac{eV\gamma}{h} \underbrace{\int dE D(E-U) \frac{f_1(E)}{2}}_N = \frac{N eV\gamma}{h}$$

$$\Rightarrow I_{ON} = \frac{N eV\gamma}{h}$$

$\alpha = CV$

For MOSFET:- (short channel)

$$I_{ON} = \frac{1}{2} \mu_m C_{ox} W [CV_{GS} - V_{TH}] E_{sat}$$

$$\text{Here } C_{ox} = \frac{EA}{d},$$

Some more terms

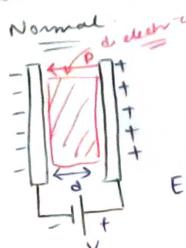
$$[CV_{GS} - V_T] \cdot \frac{V}{L} \quad \begin{cases} \text{Compare} \\ \text{Quantum capacitance} \end{cases}$$

$$\Rightarrow I_{ON} = \frac{1}{2} C_{ox} W (V_{GS} - V_{TH}) \frac{V}{L}$$

$C_Q = \alpha^2 D$

Density of states

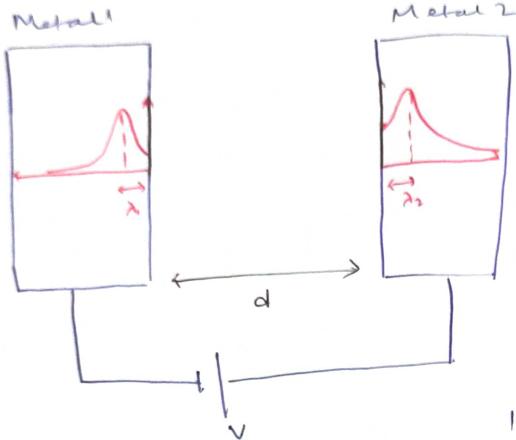
What is Quantum Capacitance?



When dielectric is inserted, polarization occurs in the dielectric. The polarization will be caused by:

- ionic Pol.
- Electronic Pol. (due to  $e^-$  cloud) → for all materials
- Dipole Pol.

When looking into charge distribution in metal plates of the capacitor, we assume they are fully on the surface, but that's actually not the case. It is actually distributed through the metal as shown below.



$$\rightarrow \text{it can be shown } (\lambda \propto \frac{dN}{dE})$$

$\lambda_1, \lambda_2 \rightarrow$  Fermi - Thomas screening length.

$$\therefore C_{\text{modified}} = \frac{\epsilon A}{d + \lambda_1 + \lambda_2}$$

$d \rightarrow$  few  $\mu\text{m}$

$\lambda_1, \lambda_2 \rightarrow$  few nm (negligible compared to  $d$ ).

So in case of large capacitors we can ignore  $\lambda_1, \lambda_2$ .

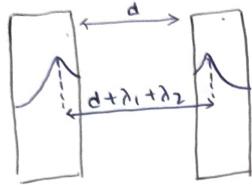
$$\therefore (C_g = \frac{\epsilon A}{d})$$

For quantum capacitance,  $d \ll (\lambda_1, \lambda_2)$  are comparable, and hence they cannot be ignored

$$\text{Geometrical Capacitance } (C) = \frac{EA}{d}$$

class - 11

$$\text{Quantum Capacitance } (C_q) = \alpha^2 D.$$



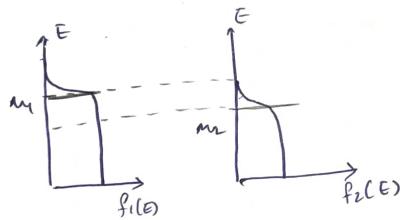
$$C' = \left( \frac{EA}{d + \lambda_1 + \lambda_2} \right)$$

if  $d \gg \lambda_1, \lambda_2$   
then the error of geometrical  
capacitance is good enough.

However, when  $d$  is comparable to  $\lambda_1, \lambda_2$ , then  
we cannot ignore them. (Here the concept of Quantum-  
Capacitance is applicable).

$\lambda_1, \lambda_2$  depends on D.S.

when  $f_1 \approx f_2 \approx f$  (The Fermi levels of the metal contacts & the S.C. are comparable)



$$f_1(E) = \frac{1}{e^{(E-\mu_1)/kT} + 1}$$

$$f_2(E) = \frac{1}{e^{(E-\mu_2)/kT} + 1}$$

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

$$\begin{aligned} \frac{\partial f}{\partial E} &= -\frac{1}{kT} \cdot \frac{1}{e^{(E-\mu)/kT}} \\ &= \frac{1}{kT} \circlearrowleft f(1-f) \end{aligned}$$

$$\mu_1 - \mu_2 = \alpha V_D$$

$$\therefore I = \alpha \int dE D(E-\mu) \frac{r}{2\pi} [f_1 - f_2]$$

$$\Rightarrow I = \alpha \int dE D(E-\mu) \frac{r}{2\pi} \left( -\frac{\partial f}{\partial E} \right) (\mu_1 - \mu_2)$$

$$\Rightarrow \frac{I}{V_D} = G = \alpha^2 \int dE D(E-\mu) \frac{r}{2\pi} \left( -\frac{\partial f}{\partial E} \right)$$

$$\Rightarrow G = \alpha^2 \int dE D(E-\mu) \frac{r}{2\pi} \frac{f(1-f)}{kT}$$

$$N = \int dE D(E-\mu) f(E)$$

N  $\approx$  1

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

$E - U \Rightarrow (\text{few } kT)$  lets say.

if lets say  $(E-U) = 10kT$

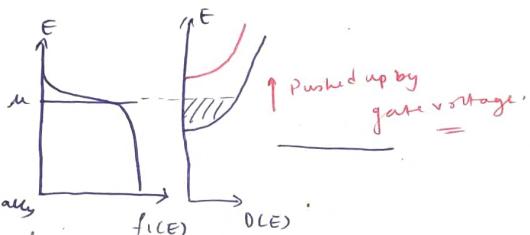
then  $f \approx e^{- (E-U)/kT}$   $\leftarrow f \text{ determines } N, \underline{\underline{G}}$ .

$$- (E-U)/kT$$

All of these vary as  $e^{- (E-U)/kT}$ . This means that while turning off a device.

When  $D(E)$  is pushed alone by a few ( $kT$ ), the conductance and current decays exponentially.

(So, the OFF state current is exponentially less compared to ON state current).



$\Rightarrow$  This is why for understanding performance of electronic device we use log scale, so comparison of OFF & ON state current can be done.

Developing the concept of Quantum Capacitance

$\therefore$  Change in the no. of  $e^-$  for change from ON to OFF state by varying gate voltage

Considering  $D(E)$  is constant  $\Rightarrow$

$$N = D_0 (U - U_g)$$

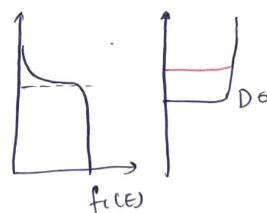
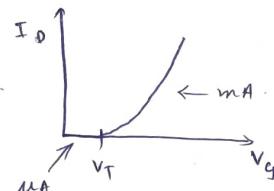
$$\Delta N = -D_0 \frac{\Delta U}{\Delta V_g} = -\alpha D_0 \Delta V_g$$

$$\Delta Q = -\alpha \Delta N$$

$$\Rightarrow \Delta Q = \underbrace{\alpha^2 D_0}_{C_Q} \Delta V_g$$

$C_Q \rightarrow$  Quantum capacitance

$$\Rightarrow \Delta Q = C_Q \Delta V_g \quad (Q = CV) \quad \underline{\underline{Q}}$$



$\Delta Q \rightarrow$  Change in charge of the channel when we switch from ON

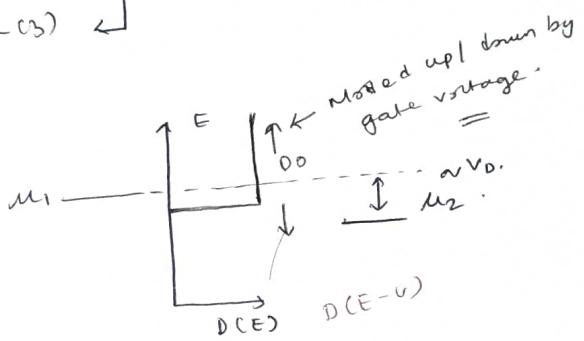
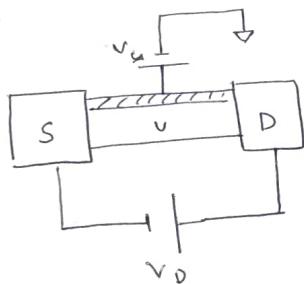
state to OFF state.

$\frac{\Delta Q}{\Delta V_g} = \frac{C_Q C}{C_Q + C}$   $\rightarrow$   $C_Q$  is other channel capacitance. Apart from  $C_Q$ , there are other capacitances involved which have smaller value. So actual change  $\Delta Q$  is lesser.

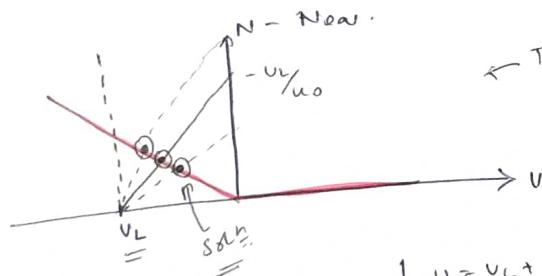
$$I = \frac{e}{h} \int dE D(E-U) \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} [f_1 - f_2] \quad (1)$$

$$N = \int dE D(E-U) \frac{f_1 \gamma_1 + f_2 \gamma_2}{\gamma_1 + \gamma_2} \quad (2) \quad \text{self consistent eqn}$$

$$U = U_L + V_0 (N - N_{eq}) \quad (3)$$



$N, U$  can be solved either computationally, or graphically.  
Let's try solving graphically.



This curve basically represents  $D(E-U)$  from the eqn (2)

$$\frac{dN}{dU} = - \left( \frac{Ca}{\omega^2} \right)$$

$$\Rightarrow \frac{dN}{dU} = C_a \quad \text{see upwards}$$

$$\Rightarrow \frac{dQ}{dV} = C_a \quad \text{see upwards}$$

$$\begin{aligned} U &= U_L + V_0 (N - N_{eq}) \\ \therefore y &= U_L + V_0 y \\ \Rightarrow y &= \frac{1}{V_0} u \left( -\frac{U_L}{V_0} \right) \\ y &= mx + c \quad \uparrow \\ y_{\text{intercept}} &= -\frac{U_L}{V_0} \end{aligned}$$

$$\frac{dN}{dU} \rightarrow \underline{\text{slope}} \quad (\text{of } N \text{ vs } U \text{ curve}) = \left( \frac{Ca}{\omega^2} \right)$$

$$V = V_L + V_0 (N - N_{\text{eq}})$$

$$\frac{dV}{dV_L} = 1 + V_0 \frac{dN}{dV_L} = 1 + V_0 \frac{dN}{dV} \cdot \frac{dV}{dV_L}$$

$$\Rightarrow \frac{dV}{dV_L} = 1 + V_0 \frac{dN}{dV} \cdot \frac{dV}{dV_L}$$

$$\Rightarrow \frac{dV}{dV_L} \left( 1 - V_0 \frac{dN}{dV} \right) = 1$$

$$V_0 = \pm \frac{a^2}{C}$$

$$\Rightarrow \frac{dV}{dV_L} = \frac{1}{1 - V_0 \frac{dN}{dV}} = \frac{1}{1 + \frac{C_\alpha}{C}}$$

$$\Rightarrow \frac{dV}{dV_L} = \frac{C}{C + C_\alpha}$$

Now, we can also find  $\frac{dN}{dV_L} = \frac{dN}{dV} \cdot \frac{dV}{dV_L}$

$$= -\frac{C_\alpha}{a^2} \cdot \frac{C}{C + C_\alpha}$$

$$\Rightarrow \frac{dN}{dV_L} \approx \left[ \frac{C_\alpha C}{C + C_\alpha} \right]$$

like series combination  
 As capacitor

# We must remember that the way we bias the source and drain contacts affect the channel potential  $V$ .

lets say:-

$V_S$	$V_D$	$V_{DS}$	Channel Potential
0	1	1	$V_1$
-1	0	1	$V_2$
-0.5	0.5	1	$V_3$

$$V_1 \neq V_2 \neq V_3$$

(Depending on the bias  
 $V_{DS}$ ,  $V$  changes so)

we must also set  $V_S$  accordingly)

# Principles of Quantum Devices:-

Unit - 13

→ The Density of states of bulk materials are found using computational techniques because it is complicated to solve analytically.

→ we can analytically solve to find DOS for simple systems such as Hydrogen atoms & Helium systems. This analytical solutions can be extended to find DOS for systems such as Graphene (2D) & Carbon NanoTube (CNT) (1D system) etc.

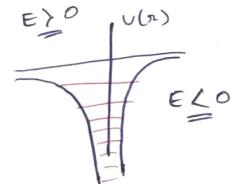
→ For solving for the DOS, we must find the E-K relation. The E-K relation is found using Schrödinger Eqn.

Schrödinger Eqn :-  $i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(r) \Psi$  ( $\Psi$  → wave function)

$$\text{Hamiltonian: } H = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \quad \begin{matrix} \text{KE} & \text{PE} \end{matrix}$$

$$\text{For Hydrogen atom: } V(r) = -\frac{Z e^2}{4\pi \epsilon_0 r} \sim \frac{1}{r}.$$

$$E_3 \longrightarrow \Psi_3 \\ E_2 \longrightarrow \Psi_2 \\ E_1 \longrightarrow \Psi_1$$



if we solve the schrödinger eqn using the  $V(r)$  for specified system. We get the wave  $\Psi$

let  $V=0$  (free p'cle).

$$\Psi = A e^{-iEt/\hbar} e^{ikx}$$

Then soln of schrödinger eqn :-

$$\text{Haw! } \underset{=} {V=0} \quad i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi \quad \overset{\frac{\partial^2}{\partial x^2} (1-D)}{=}$$

$$\text{Solv.} \quad \Rightarrow i\hbar \left( -\frac{iE}{\hbar} \right) \Psi = -\frac{\hbar^2}{2m} (ik)^2 \Psi \quad \begin{matrix} \text{m} \rightarrow \text{mass} \\ \text{p'cle} \end{matrix}$$

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

$$E = \frac{\hbar^2 k^2}{2m} \quad (\text{is the Energy of a free electron}).$$

continuous Energy level

→ This E-K relation is called the Dispersion relation!

if we consider 2 dimensions:-

Schrödinger Eqn:-

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial y^2}$$

Solution for free space  $U=0$

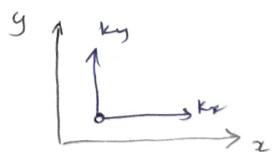
$$\Rightarrow \Psi = A e^{-iEt/\hbar} \cdot e^{ik_xx} \cdot e^{ik_yy}$$

why are we multiplying?

→  $\Psi$  gives probability of finding the particle so the joint probability will be multiplication of the individual probabilities.

Here, if we solve for E, then we get the E-K relation!-

$$E = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m}$$



For solving for D.O.S., we generally do not consider the time

dependent part of the Schrödinger Eqn:-

$$\Psi(x, t) = \underline{\Phi(x)} \cdot \underline{\Phi(t)} \text{ we ignore}$$

gives us D.O.S.

Time independent Schrödinger Eqn :-

$$E \psi(r) = -\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r) \psi(r).$$

$\Rightarrow$  Now if we have a hydrogen atom, we put  $V(r) = -\frac{ze^2}{4\pi\epsilon_0 r}$ .  
 $(z=1)$

If we find the  $\psi(r)$  & some for E, we get:-

$$\boxed{E = -\frac{E_0}{n^2}}$$

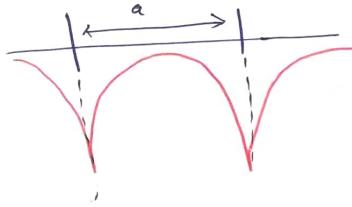
$$n = 1, 2, 3, \dots$$

$$E_0 = 13.6 \text{ eV}$$

$\rightarrow$  Till now what we have seen is the analytical soln of differential Eqn for finding  $\psi$  & E. However if we have a complicated  $V(r)$ , then instead of solving purely analytically, we use some semi-empirical techniques to solve the system & find  $\psi$  & E.

Let's say for H-molecule! -

$$V(r) = \sum_{i=1}^n V_i(r) . \text{ For } H_2 \text{ atom}$$



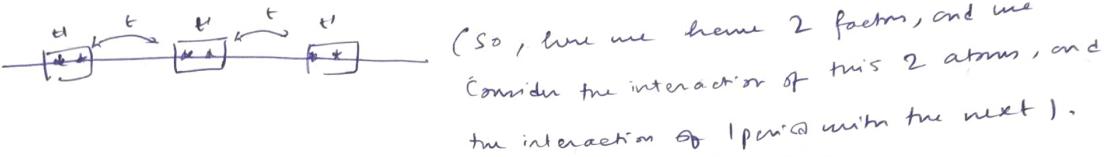
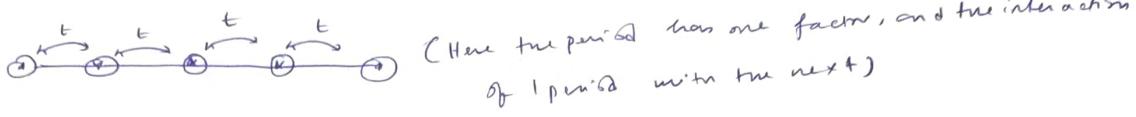
For extremely large n, let's say  $\frac{n^2}{a} \approx \infty$ .

$$V(r) = \sum_{i=1}^{\infty} V_i(r) \leftarrow \begin{array}{l} \text{when we solve for } V(r), \text{ the soln will} \\ \text{have a factor of } \frac{1}{a}. \text{ (distance b/w atoms).} \end{array}$$

Once we have solved for  $V(r)$ , we can solve Schrödinger Eqn for  $E \psi = H \psi$ .

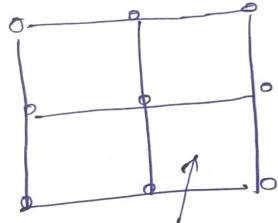
$E \psi = H \psi$ . (However this will take years for generating soln even by best computational facilities.)

So, we introduce some simple fixations to estimate the soln efficiently.



$$\psi(n) = \sum_n U_n \underbrace{U(n)}_{\substack{\text{Basis } f_n \\ \equiv}} \quad \left| \begin{array}{l} \text{Time independent} \\ \text{Schrödinger Eqn.} \end{array} \right.$$

$$E\psi(n) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + U \right] \psi(n).$$



we find the Basis  $f_n$  for 1 atom, and then 1 atom  
find the period in  $x$  &  $y$  direction & solve for  $\psi(n)$  in form  
of matrix.

$$E \{ \psi \} = \begin{bmatrix} I_t \end{bmatrix}_{n \times n} \{ \psi \}$$

↑ includes potential info.  
=

$$\Rightarrow E [s] \{ \psi \} = \begin{bmatrix} I_t \end{bmatrix}_{m \times n} \{ \psi \}$$

↑ unit matrix

$$H_{mn} = \int d^3 r \underbrace{U_m H_{mn} U_n}_{=}$$

$$S_{mn} = \int d^3 r U_m U_n$$

Let's take Example for  $H_2$  molecule.

$$H_{mn} = \begin{bmatrix} \epsilon & t \\ t & \epsilon \end{bmatrix}$$

$H$  —————  $H$

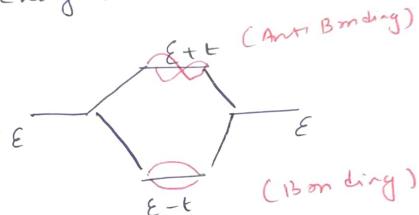
interaction of 2 H atom ( $\epsilon$  both off diagonal elements taken same  $\rightarrow$  assuming same interaction b/w the 2 H atoms).

Energy of 1 H<sub>2</sub> hydrogen atom.

(Diagonalize this gives us the Energies.)

$$E_1 = (\epsilon + t)$$

$$E_2 = (\epsilon - t)$$



This concept is extended for graphite to find the D.O.S.

From Schrödinger Equation (Time independent).

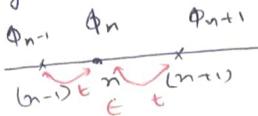
$$E \Phi(x) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V \right] \Phi(x)$$

}  $\rightarrow$  we can solve  
analytically or numerically.

$$\Phi(x) = \sum_n \Phi_n u_n(x)$$

If we write this in matrix form, we will get: - (for group of atoms)

$$E \{ \Phi_n \} = [H] \{ \Phi_n \}$$



$$[H] = \begin{bmatrix} E & t & t & & \\ t & E & t & & \\ t & t & E & & \\ & & & \ddots & \\ & & & & \dots \end{bmatrix}$$

$t$   
 $\downarrow$   
 $\text{in } (ka)$

$$\Phi_n = \Phi_0 e^{inx}$$

Solution of the Schrödinger Eqn gives us this.

Diagonal elements give self interaction  
Off diagonal terms gives us the interaction between  
different atoms. (All t's are considered same  
because all atoms are  
same & positioned  
arranged).

$k \rightarrow$  wave vector  
 $a \rightarrow$  distance b/w atoms

writing the matrix terms,

$$E \begin{Bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{Bmatrix} = \begin{bmatrix} E & t & t & \cdots & t \\ t & E & t & \cdots & t \\ t & t & E & & \\ \vdots & & & \ddots & \\ t & t & \cdots & & E \end{bmatrix} \begin{Bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{Bmatrix}$$

$$\therefore E \Phi_n = t \Phi_{n-1} + t \Phi_n + t \Phi_{n+1}$$

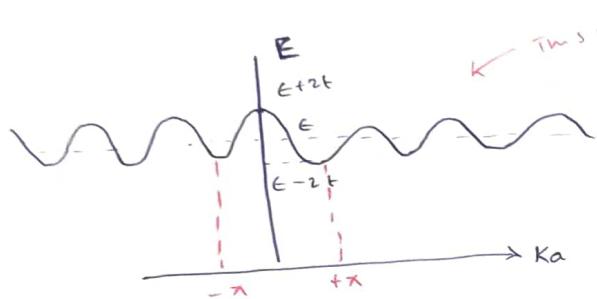
{ if we put  $\Phi_n$  in this equation, we can solve  
for the energy as:-  
 $\Phi_n = \Phi_0 e^{inx}$  }

$$\Rightarrow E \Phi_0 e^{inx} = t \Phi_0 e^{inx} + E \Phi_0 e^{inx} + t \Phi_0 e^{inx}$$

$$\Rightarrow E = \underbrace{t e^{inx}}_{-ika} + E + \underbrace{t e^{inx}}_{ika} = E + 2t \cos(ka)$$

$$\Rightarrow E = E + 2t \cos(ka)$$

$E$  varies b/w  $E+2t$  &  $E-2t$ .



This is like the E-E relation  
if we use periodic boundary  
cond  $\frac{N}{a}$ , then

$$\phi_N = \phi_1$$

$\equiv$

$iN(ka)$

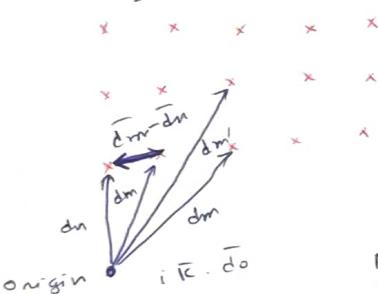
$$\phi_N = \phi_0 e^{iN(ka)}$$

$$\phi_1 = \phi_0 e^{i(2\pi)} \\ \therefore e^{iN(ka)} = 1 = e^{i(2\pi)}$$

$$\Rightarrow K_a = \frac{2\pi}{N}$$

$\sim\!\!\!\sim\!\!\!\sim$

For 2D



For 1D



$$\phi_n = \phi_0 e^{iK \cdot \bar{d}n}$$

$\equiv$

For 2D

$$i\bar{K} \cdot \bar{d}n = \sum_m H_{nm} e^{i\bar{K} \cdot \bar{d}m}$$

$$E \phi_0^2$$

$$\Rightarrow E = \sum_m H_{nm}^2$$

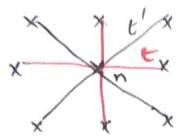
$\sim\!\!\!\sim\!\!\!\sim$

$i\bar{K} \cdot (\bar{d}m - \bar{d}n)$  ← more general (dimension independent form).

$(\bar{d}m - \bar{d}n)$  is equivalent to lattice parameter  $a$ .

Gives the Energy  
due to interaction of  $n$  atom with  
 $m$  nearby atoms.

HW



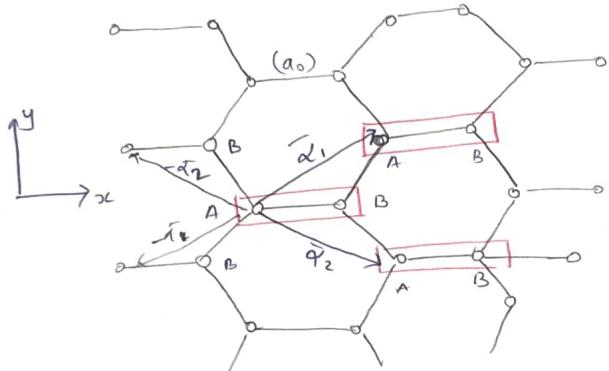
$$E = \sum_m H_{nm} e^{i\vec{k}(\vec{d}_m - \vec{d}_n)}$$

Write down the Energy

expression of this in matrix form :-

→ Calculate  $H_{nm}$  first, and then sum for  $E$ .

Graphene structure :-



Bond length  $a = \underline{\underline{a_0}}$

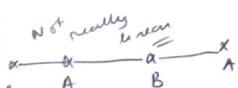
Find angle b/w the terms.

Find expression for  $\vec{\alpha}_1$  &  $\vec{\alpha}_2$  in terms of  $a_0$ .

The next element of the ~~graphene~~ Graphene is the 2 carbon system. If translated properly, will form the whole structure.

$$\vec{\alpha}_1 = \hat{x} \cdot \frac{3a_0}{2} + \hat{y} \cdot \frac{\sqrt{3}a_0}{2}$$

$$\vec{\alpha}_2 = \hat{x} \cdot \frac{3a_0}{2} - \hat{y} \cdot \frac{\sqrt{3}a_0}{2}$$



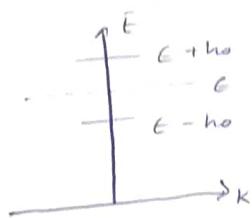
$$h(\vec{k}) = \begin{bmatrix} \epsilon & t \\ t & \epsilon \end{bmatrix} + \begin{bmatrix} e^{i\vec{k} \cdot \vec{\alpha}_1} \\ e^{-i\vec{k} \cdot \vec{\alpha}_1} \end{bmatrix} + \begin{bmatrix} e^{i\vec{k} \cdot \vec{\alpha}_2} \\ e^{-i\vec{k} \cdot \vec{\alpha}_2} \end{bmatrix}$$

$$h(\vec{k}) = \begin{bmatrix} \epsilon & \omega_0 \\ \omega_0 & \epsilon \end{bmatrix} + \begin{bmatrix} e^{-i\vec{k} \cdot \vec{\alpha}_1} \\ e^{-i\vec{k} \cdot \vec{\alpha}_2} \end{bmatrix}$$

$$\omega_0 = t \left( 1 + e^{-i\vec{k} \cdot \vec{\alpha}_1} + e^{-i\vec{k} \cdot \vec{\alpha}_2} \right)$$

$$E = \epsilon \pm i\omega_0$$

$$\bar{\epsilon} = \epsilon \pm 1 \text{ ns}$$



$$E\phi = \left( -\frac{\hbar^2}{2m} \nabla^2 + U \right) \phi$$

$$E\{\phi\} = [H]\{\phi\}$$

N by N  $\xrightarrow{\text{matrix}}$   
 v. large

$N \rightarrow \text{No. of unit cell}$   
 $b \rightarrow \text{no. of atoms per unit cell}$   
 (basis  $P^n$ )

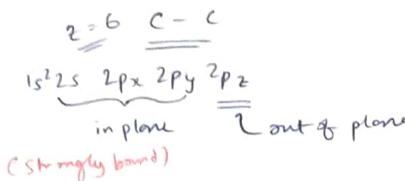
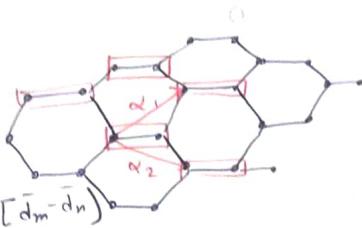
$$E\{\phi_n\} = \sum_m [H_{nm}] \phi_m$$

(difficult  
to diagonalize)

$$[H]\{\phi\} = E\{\phi\}$$

$b \times b$   
 smaller matrix of order  
 the basis

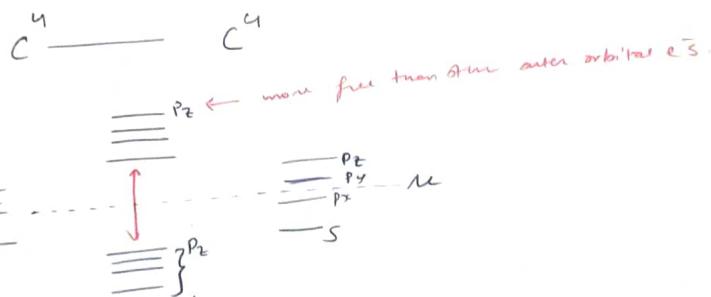
$$h(K) = \sum_m [H_{nm}] e$$



(We are interested in  $2p_z$  orbital because it's nearest to the chemical potential).

For graphene  
repeatable unit

$\alpha_1$ ,  $\alpha_2 \rightarrow$   
 translation  
unit vectors  
 $\vec{s} = m\vec{\alpha}_1 + n\vec{\alpha}_2$



The no. of basis function does not depend on the no. of atoms / unit cell. But it actually depends on the electronic configuration of the atoms and see how many levels one is interested in.

$$\bar{\alpha}_1 = \hat{x} \frac{3a_0}{2} + \hat{y} \frac{\sqrt{3}a_0}{2}$$

$$\bar{\alpha}_2 = \hat{x} \frac{3a_0}{2} - \hat{y} \frac{\sqrt{3}a_0}{2}$$

for Graphene

unit vectors

$a = \frac{3}{2}a_0$

$b = \frac{\sqrt{3}}{2}a_0$

$= \hat{x}a + \hat{y}b$

$\hat{x}a - \hat{y}b$

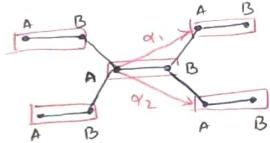
$a = \sqrt{3}b$

$$h(k) = \begin{bmatrix} A & B \\ B & A \end{bmatrix} e^{i\vec{k} \cdot \bar{\alpha}_1} + \begin{bmatrix} A & B \\ B & A \end{bmatrix} e^{i\vec{k} \cdot \bar{\alpha}_2}$$

unit cell

$$+ \begin{bmatrix} A & B \\ B & A \end{bmatrix} e^{-i\vec{k} \cdot \bar{\alpha}_1} + \begin{bmatrix} A & B \\ B & A \end{bmatrix} e^{-i\vec{k} \cdot \bar{\alpha}_2}$$

P  
neighbors



$$h(k) = \begin{bmatrix} \epsilon & t(1 + e^{i\vec{k} \cdot \bar{\alpha}_1} + e^{-i\vec{k} \cdot \bar{\alpha}_2}) \\ t(1 + e^{i\vec{k} \cdot \bar{\alpha}_1} + e^{i\vec{k} \cdot \bar{\alpha}_2}) & \epsilon \end{bmatrix}$$

$$h(k) = \begin{bmatrix} \epsilon & h_0 \\ h_0^* & \epsilon \end{bmatrix} \quad h_0 = t(1 + e^{-i\vec{k} \cdot \bar{\alpha}_1} + e^{-i\vec{k} \cdot \bar{\alpha}_2})$$

$$\text{The } \vec{k} \text{ vector has } \Rightarrow \vec{k} = k_x \hat{x} + k_y \hat{y}$$

$$\therefore \bar{\alpha}_1 = a k_x + b k_y$$

$$\bar{\alpha}_2 = a k_x - b k_y$$

using this

$$h_0 = t(1 + e^{-ikxa} e^{-ikyb} + e^{-ikxa} e^{ikyb})$$

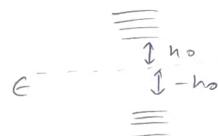
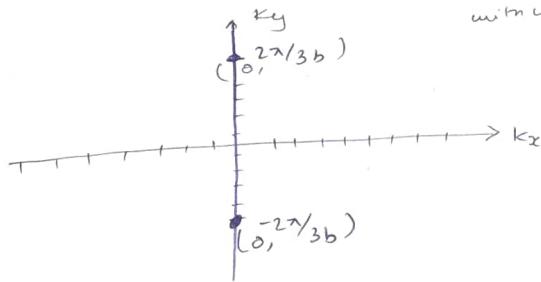
$$\Rightarrow h_0 = t \left\{ 1 + e^{-ikxa} \left( \frac{e^{-ikyb} + e^{ikyb}}{2} \right) \right\}$$

$$h_0 = t \left\{ 1 + 2 e^{-ik_x a} \cos(k_y b) \right\}$$

So, the Energy splitting around  $E$  would be  $\begin{bmatrix} E + h_0 \\ E - h_0 \end{bmatrix}$

$E \rightarrow$  chemical potential for graphene.

(Each  $e^-$  has a specific  $\vec{k}$  value) with which it travels. It is important to remember that  $\vec{k}$  values are discrete.



We are interested around  $E$ , so we have to see

where  $h_0$  values are 0

$$h_0 = 0 = t \left\{ 1 + 2 \underbrace{\sin}_{1} \underbrace{\cos}_{-1/2} (k_y b) \right\}$$

$k_x a = 0$  } two pts in k-space act near Fermi Energy.  
 $k_y b = \pm \frac{2\pi}{3}$  }  
 $\pi$  =

Some are interested only in these two points which are near  $E$ .

$\therefore k_x = 0$   
 $\Rightarrow k_y = \pm \frac{2\pi}{3b}$

$k$  values of interest

$\equiv$   
 $\equiv$   
 $\equiv$

We will expand  $h_0$  near the two valleys to see how  $e^-$ 's behave near the valleys (By Taylor series)

$$h_0(k_x, k_y) = h_0 \left( 0, \frac{2\pi}{3b} \right) + \frac{\partial h_0}{\partial k_x} \Big|_{0, \frac{2\pi}{3b}} (k_x - 0) + \frac{\partial h_0}{\partial k_y} \Big|_{0, \frac{2\pi}{3b}} (k_y - \frac{2\pi}{3b})$$

$$\frac{\partial h_0}{\partial k_x} \Big|_{0, \frac{2\pi}{3b}} = 2t (-i \frac{\partial}{\partial a}) e^{-ik_x a} \Big|_{-1/2} \cos(k_y b) = -i a t$$

$$\frac{\partial h_0}{\partial k_y} \Big|_{0, \frac{2\pi}{3b}} = -2t \frac{e^{-ik_x a}}{b} \Big|_{-1/2} \sin(k_y b) = -\sqrt{3} b t$$

$$h_0(k_x, k_y) = h_0(0, \frac{2\pi}{3b}) + \left. \frac{\partial h_0}{\partial k_x} \right|_{0, \frac{2\pi}{3b}} (k_x - 0) + \left. \frac{\partial h_0}{\partial k_y} \right|_{0, \frac{2\pi}{3b}} (k_y - \frac{2\pi}{3b})$$

$$h_0(k_x, k_y) = 0 - i\alpha t k_x - \sqrt{3} b t (k_y - \frac{2\pi}{3b})$$

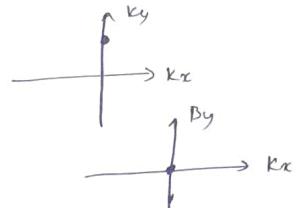
$$\Rightarrow h_0(k_x, k_y) = -i\alpha t \left( k_x + \frac{\sqrt{3}b}{\alpha} (k_y - \frac{2\pi}{3b}) \right)$$

$\alpha = \sqrt{3}b$   
 $b/a = \frac{1}{\sqrt{3}}$

$$\Rightarrow h_0(k_x, k_y) = -i\alpha t \left( k_x - i(k_y - \frac{2\pi}{3b}) \right)$$

$$\Rightarrow h_0(k_x, k_y) = -i\alpha t (k_x - i\beta_y)$$

$$\beta_y = k_y - \frac{2\pi}{3b}$$

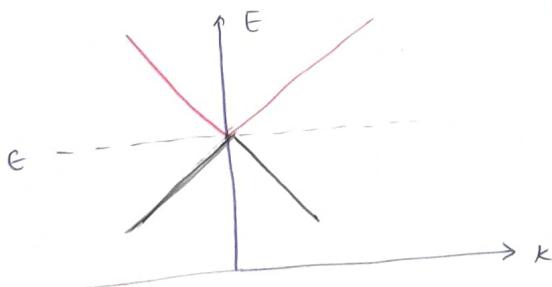


$$E = \epsilon \pm |h_0|$$

$$\Rightarrow E = \epsilon \pm at \sqrt{k_x^2 + \beta_y^2}$$

E-K relation for graph hence

$$\text{plotting E-K: } E = \epsilon \pm \text{at } K \quad (\text{Dispersive E-K relation})$$



(using this we can find density of states as -)

$$D(E) = \sum_k \delta(E - E(k))$$

$\Delta E = \frac{h^2}{m}$

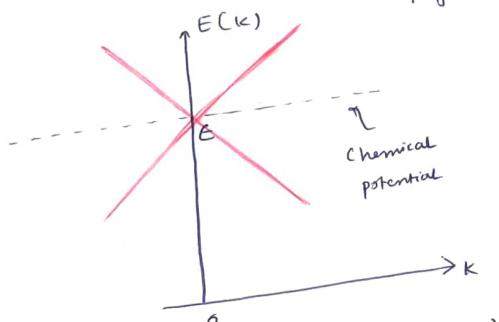
Schrodinger Eq<sup>n</sup>

$$E \psi(x) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] \psi(x)$$

For graphene, we find :-

$$E(k) = E \pm at \sqrt{k_x^2 + \beta_y^2} = E \pm atk$$

$$\beta_y = \frac{ky - 2\pi}{3b}$$



(Dispersion relation for graphene.)

→ Linear E-K relation

Let us calculate N for Graphene.

$$N = \int D(E) f(E) dE$$

(K → discrete K values, we calculate N around fermi Energy. Not from  $-\infty$  to  $\infty$ )

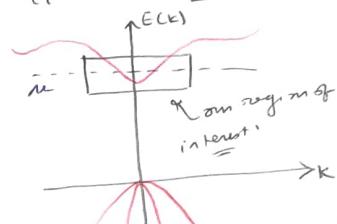
$$\Rightarrow N = \sum_k f(E(k))$$

Summation of probability of occupancy of a state  $E(k)$  gives us no. of e<sup>-</sup>s.

At  $k_1 \rightarrow E(k_1) \rightarrow f_0(E(k_1))$   
 $k_2 \rightarrow E(k_2) \rightarrow f_0(E(k_2))$   
 $k_3 \rightarrow E(k_3) \rightarrow f_0(E(k_3))$

Gives probabilities

Previously, we have seen for bulk solids :- (Parabolic E-k relation).



Approximation around Fermi Energies :-

$$E(k) = E_c + \frac{\hbar^2 k^2}{2m}$$

constant  $\approx$  is treated as a parameter to fit our free E-k relation

we have seen the energy from free pde.

(This means e<sup>-</sup>s in a bulk S.C. near band edge behave like free electrons, however the mass will be → effective mass)

We know  $\int_{-\infty}^{\infty} f(x) \delta(x-a) dx = f(a)$

If  $= 0$ , not occupied.  
 If  $= 1$ , e<sup>-</sup> present.

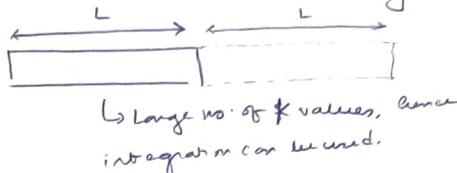
$$N = \int dE D(E) f(E) \quad \text{if } D(E) = \delta(E - E(k))$$

$$\Rightarrow N = \int dE \delta(E - E(k)) f(E) = f(E_k)$$

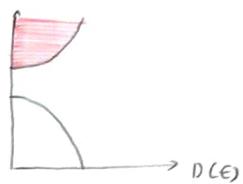
$$\text{For various } k \text{ values: } D(E) = \sum \delta(E - E(k))$$

$$\Rightarrow N = \sum f(E(k))$$

For large sample



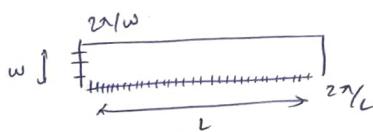
We can convert the summation to integration if we have large no. of  $k$ ,  
and they are closely spaced



$$\text{Minimum value of } k, \text{ i.e. } (k = \frac{2\pi}{L})$$

(Separation b/w 2 Energy levels  $\approx \frac{\Delta E}{2}$ )

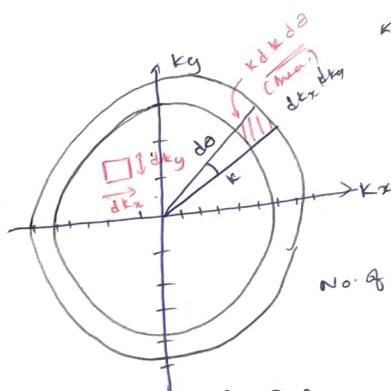
if  $L$  is large,  $k$ 's are nearly close to each other  $\rightarrow$  almost continuous



Density of states is a summation of  $\delta$  functions,

$D(E) = \sum \delta(E - E(k))$ , i.e. There is a state for  $e^-$  whenever  $E = E(k)$ .

For 2 D materials:-



NO. OF  $k$  VALUES IN LENGTH  $dk_x = \frac{2\pi}{2\pi/L} dk_x$

Spacing of  $k$  in  $x$  by directions depend on dimensions in  $x$  by direction.

$$dk_y = \frac{dk_y}{2\pi/w}$$

$$D(E) = \iint \frac{dk_x}{2\pi/L} \frac{dk_y}{2\pi/w} \delta(E - E(k))$$

$$= \frac{LW}{4\pi^2} \iint dk_x dk_y \delta(E - E(k))$$

For a symmetric solid,  $L = \underline{w}$

$$D(E) = \frac{L \cdot w}{4\pi^2} \iint \frac{dk_x dk_y \delta(E - E(k))}{d\theta} \quad \text{Replace by } k dk d\alpha$$

$$D(E) = \frac{S}{4\pi^2} \iint k dk d\alpha \delta(E - E(k)) \quad S = \underline{\underline{Lw}}$$

$$\Rightarrow D(E) = \frac{S}{4\pi^2} \iint_{\frac{\pi}{2\pi}} k \delta(E - E(k)) dk = \frac{S}{2\pi} \int k \delta(E - E(k)) dk.$$

For graphene  $E(k) = E \pm atk$        $\left. \begin{array}{l} \\ \end{array} \right\} \text{Replace variable } dk \text{ by } \frac{dE}{at}$   
 $dk = at dk$        $\left. \begin{array}{l} \\ \end{array} \right\} \text{dE} = at dk$

$$\Rightarrow D(E) = \frac{S}{2\pi} \int \frac{E(k)}{at} \delta(E - E(k)) \cdot \frac{dE(k)}{at} \quad \text{For delta f.} \quad \delta(x-a) = \delta(a-x)$$

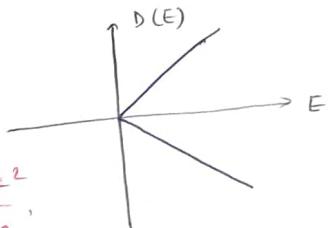
$$\Rightarrow D(E) = \frac{S}{2\pi a^2 t^2} \int E(k) \delta(E(k) - E) dE(k)$$

$$\Rightarrow D(E) = \frac{S}{2\pi a^2 t^2} \int_{-\infty}^{\infty} x \delta(x - E) dx$$

$$\Rightarrow D(E) = \frac{S}{2\pi a^2 t^2} |E|$$

H.W. calculate  $D(E)$  as a solt with  $E(k) = \frac{\hbar^2 k^2}{2m}$ ,

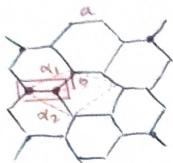
Density of states for  
Graphene



# Principles of Quantum Devices

Atom - 17

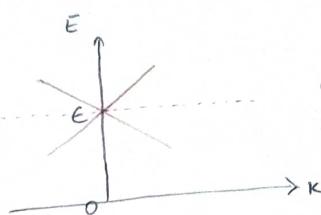
## Graphene



Chemical potential

$$E(k) = E + \alpha t \sqrt{k_x^2 + \beta y^2} \approx E + \alpha t k$$

$$\beta y = ky - \frac{2\pi}{3b}$$



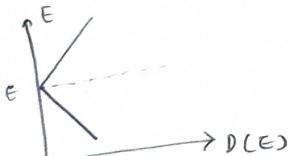
We can calculate D.O.S. from  $E(k)$  → done in last class.

$$N = \int dE D(E) f_0(E) \Rightarrow \text{Sampling theorem.}$$

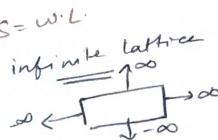
$$D(E) = \sum_k S(E - E(k))$$

$$\Rightarrow D(E) = \int \frac{dk_x}{2\pi/L} \frac{dk_y}{2\pi/W} S(E - E(k)) \quad E(k) = \text{at } |k|$$

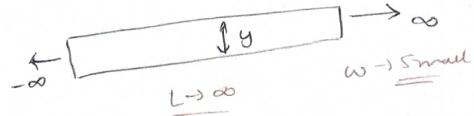
$$\Rightarrow D(E) = \frac{LW}{4\pi^2} \int d\theta \int k dk S(E - E(k))$$



$$\Rightarrow D(E) = \frac{S}{2\pi} \frac{|E|}{a^2 E^2} \quad \text{for infinite lattice}$$



lets restrict along one direction. (y).  
K confinement effect in y direction.



$$E(k) = E + \alpha t \sqrt{k_x^2 + \beta y^2}$$

$$D(E) = \sum_{k_x, k_y} S(E - E(k))$$

$$\Rightarrow D(E) = \frac{L}{2\pi} \sum_{ky} \int dk_x S(E - E(k))$$

$k_y \rightarrow \infty$  infinitesimally small.  
Keep  $\alpha t \sum$ . (Find  $dk_x$  from  $E(k)$ )

$$D(E) = \frac{L}{2\pi \alpha t} \sum_{ky} \int dE \cdot \frac{E}{\sqrt{E^2 - \alpha^2 t^2 + \beta y^2}} S(E - E(k))$$

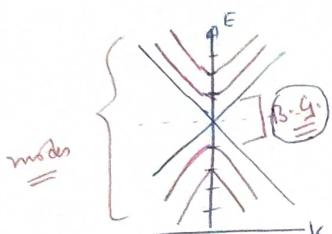


$k_x \rightarrow$  infinitesimally small. But  $k_y \rightarrow \infty$  infinitesimally small.  
Keep  $\alpha t \sum$ .

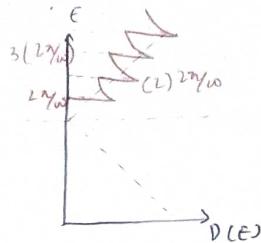
$$\Rightarrow D(E) = \frac{L}{2\pi \alpha t} \sum_{ky} \frac{E}{\sqrt{E^2 - \alpha^2 t^2 + \beta y^2}}$$

D.O.S. of a thin graphene sheet

D.O.S. of this thin graphene sheet :-



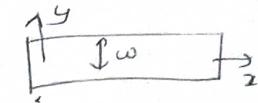
B.G. created when graphene sheet is made thin.



$$\beta_g = \frac{2\pi}{\omega} \nu$$

$\nu \rightarrow \underline{\text{integer}}$

$$D(E) = \frac{L}{2\pi a^2} \sum_{k_y} \left[ \frac{E}{\sqrt{E^2 - a^2 k_y^2 \beta_g^2}} \right]$$



# If we cut the sheet in a particular way so that the properties of one edge is same as the other edge. Then if we roll it in a tube form, we get a periodic B.C. & thus, we get a carbon nanotube (if  $\omega \rightarrow$  look into periodic B.C. and Box B.C.)

( $\underline{\text{if } \omega}$ )

# Wrapping along  $x$  direction.  
(Repetitive unit dimension =  $2a$ ).

$$E_\nu(k_y) = \pm \text{at } \sqrt{k_y^2 + \beta_g^2}$$

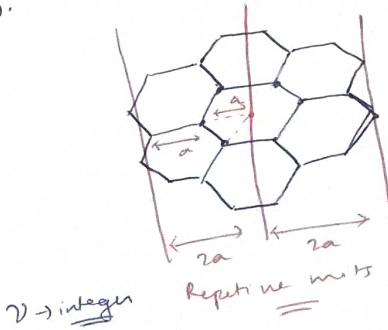
Wrapping along  $x$  axis !

$$k_y(2a \cdot m) = 2\pi \nu$$

(quantization coefficient)

$$k_y = \frac{2\pi}{2am} \nu$$

How :- Calculate D.O.S when graphene is wrapped around  $y$  axis.



$\nu \rightarrow \underline{\text{integer}}$

Repetitive units

$\sim D(E) = \frac{L}{2\pi a^2} \sum_{k_y} \left[ \frac{E}{\sqrt{E^2 - a^2 k_y^2 \beta_g^2}} \right]$

Solve  $\underline{\text{m}^3}$  integral.

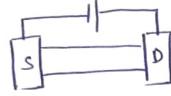
$$D(E) = \frac{L}{2\pi a^2} \sum_{k_y} \left[ \frac{E}{\sqrt{E^2 - a^2 k_y^2 \beta_g^2}} \right]$$

# The properties of the C.N.T. depend on how we are rolling / wrapping the graphene sheet. It can be  $\begin{cases} \text{metallic (C.N.T. B.G.)} \\ \text{S.C. (B.G. } \sim 3\text{ eV)} \\ \text{Single wall CNT} \end{cases}$  we will also see density of states M(E).

# Principles of Quantum Devices :-

class - 18

We have previously seen:-



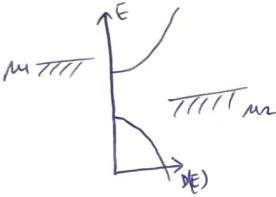
$$D(E) = \sum_k S(E - E(k))$$

$$I = \frac{a}{h} \int dE D(E) \left[ \frac{\tau_1 \tau_2}{\tau_1 + \tau_2} \right] [f_1 - f_2]$$

↑  
current through one  
channel.

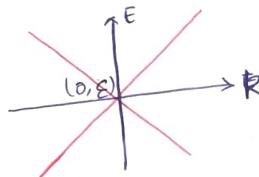
$$N = \int dE D(E) f(E)$$

$$\text{where } f(E) = \left[ \frac{\tau_1 f_1 + \tau_2 f_2}{\tau_1 + \tau_2} \right]$$

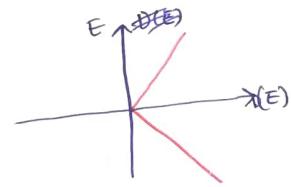


For Graphene :- (infinite sheet)

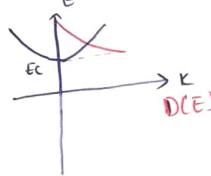
Dispersion relation



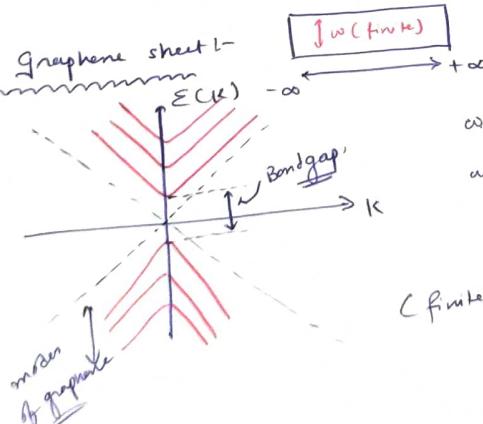
Density of States :-



P previously seen :- (For parabolic E-K relation) :-



For finite Graphene sheet :-

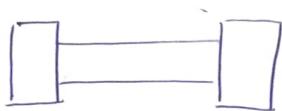
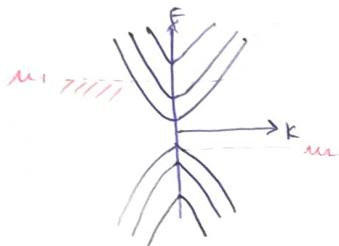


when making C.N.T. from graphene,  
we have to cut it in an apt. manner.

(finite graphene has multiple modes).

If graphene is used in the device:-

(!! we are using E-k relation instead of D(E) graph !!) ← Assumption



(more no. of modes enclosed b/w  $E_1$  &  $E_2 \rightarrow$   
more no. of channels → more current).

Since now, the current not only depends on the density of states but also on how closely the modes are located in Energy, we define another parameter on which the current depends → Density of modes ( $M(E)$ )

We define D.O. Modes as follows:-

$$M(E) = \sum_k \delta(E - E(k)) \left[ \frac{\pi v_x \sqrt{v_x(E)}}{L} \right]$$

we have previously defined Quantum conductances as!:-

$$G = \frac{e^2}{h} (\pi D) \underset{\text{integer}}{\cancel{}}$$

But, when we have modes, we can redefine the quantum conductance expression as!:-

$$G = \frac{e^2}{h} (M) \underset{\text{integer (coming from Density of modes)}}{\cancel{}}$$

we can find no. of Electrons in a system as!:-

$$N = \sum_k f_0(E(k)) \xrightarrow{\text{how?}} -$$

$$\begin{aligned} N(E) &= \int dE D(E) f_0(E) \\ &= \int dE \sum_k \delta(E - E(k)) f_0(E) \\ &= \sum_k f_0(E(k)) \end{aligned}$$

Also, the current!-  $\downarrow$  velocity

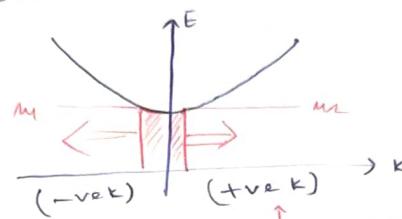
$$I = \frac{ev}{L} \sum_k f_0(E(k)) \cdot v(k) \xrightarrow{\text{from no. of es.}}$$

$$I = \frac{nq}{T}$$

$$I = \frac{e}{L} \sum p_0(E(k)) \cdot v(k).$$

so, velocity plays an important role.

# If we look at the  $E(k)$  relation! -

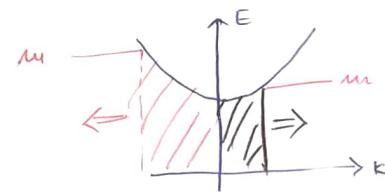


Corresponds to e^-'s moving in opposite directions.

Corresponds to e^- moving in one direction

At equilibrium, these two effects are equal and cancel each other.

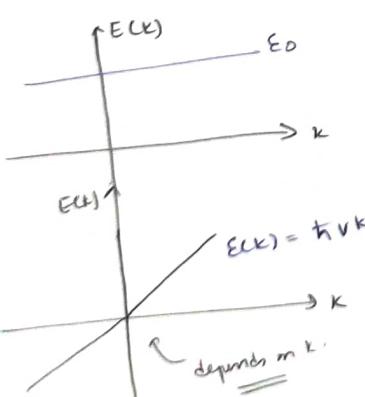
At non equilb., no. of e^-'s moving in opposite directions are not equal, and there is an effective current.



Now, how does the velocity of e^-'s determined.

The wave eqn. of the e^-'s:-

$$\Psi = \sum_K C_K e^{iKx} e^{-i\frac{E(K)t}{\hbar}}$$



So, electrons move with velocity v.

$$\Psi = \sum_K C_K e^{iKx} e^{-i\frac{E_0 t}{\hbar}}$$

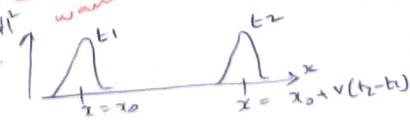
constant  $E-K$ .  
So, e^-'s have no velocity. They do not move with time.  
no dependence on  $K$

$$\Psi \sim e^{iKx} e^{-i\frac{E_0 K t}{\hbar}}$$

$$\Psi \sim e^{iKx} e^{-i(vKt)}$$

$$\Psi \sim e^{i(x-vt)} e^{-i(vKt)}$$

Eav. for travelling wave.



So, we define velocity of  $e^-$  as :-

$$\bar{v}(k) = \frac{1}{\hbar} \nabla_k E(k)$$

For any  $k$  direction :-

$$v(k_x) = \frac{1}{\hbar} \frac{\partial E}{\partial k_x}$$

So, rewriting the current eqn in terms of Density of modes :-

$$I = \frac{ev}{\hbar} \int d(E) \underline{M(E)} (f_1(E) - f_2(E))$$

$M(E) f_1(E) \rightarrow$  gives current in right direction.

$M(E) f_2(E) \rightarrow$  gives current in left direction.

So how is  $M(E)$  connected to  $D(E)$ ?

$$D = I S(E - E(k))$$

$$M = \pi D \frac{\hbar v_x}{L}$$

$$D(E) = \sum_k S(E - E(k))$$

$$N = \int dE D(E) f(E)$$

$$M(E) = \sum_k S(E - E(k)) \frac{\pi n |v_x(k)|}{L} \quad \left\{ v_x(k) = \frac{1}{\hbar} \frac{\partial E(k)}{\partial k_x} \right.$$

$$I = \frac{e}{\hbar} \int dE M(E) (f_1(E) - f_2(E)) \quad \text{Both should give some current!}$$

$$I = \frac{e}{\hbar} \int dE D(E) \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (f_1(E) - f_2(E)) \quad \left\{ \text{if } \gamma_1 = \gamma_2, \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} = \frac{\gamma^2}{2} \right\}$$

$$N = \int dE D(E) \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

Making denominator  $\hbar$

$$I = \frac{e}{2\pi\hbar} M(E) = \frac{1}{\hbar} D(E) \frac{\gamma}{2}$$

$$\frac{1}{n} M(E) = \frac{2\pi}{\hbar} D(E) \frac{\gamma}{2}$$

$$M(E) = \pi D(E) \frac{\gamma}{2}$$

Quantum conductance :-

$$G_q = \frac{e^2}{\hbar} (\pi D \frac{\gamma}{2}) = \frac{e^2}{\hbar} M \quad \text{integer}$$

Let's study a specific case :-

$$E(k) = \frac{\hbar^2}{2m} (k_x^2 + k_y^2)$$

$L \rightarrow$  infinitely large

$w \rightarrow$  small

$$\begin{aligned} \therefore k_x &= \frac{2\pi}{L} \rightarrow \text{very small} \\ \therefore k_y &= \frac{2\pi}{w} \rightarrow \text{large} \end{aligned} \quad \left\{ \begin{array}{l} \text{Periodic boundary} \\ \text{cond} = \frac{2\pi}{L} \end{array} \right.$$

$$\text{For Box Boundary cond} = \frac{2\pi}{L}$$

$$k = \frac{2\pi}{L}$$

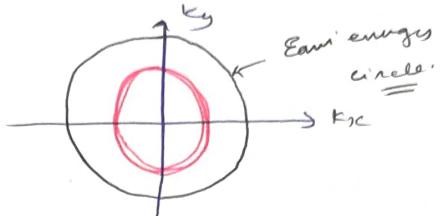
For Box Boundary condition :-

$$k_{yn} = n \frac{\pi}{L}$$

$$\epsilon(k) = \frac{\hbar^2}{2m} (k_x^2 + k_y^2)$$

Periodic Boundary condition :-

$$k_{yn} = n \frac{2\pi}{L}$$



$k_x \rightarrow$  continuous  
 $k_{yn} \rightarrow$  discrete

For such a system :-

$$\therefore M(E) = \sum_{k_x} \sum_{k_y} \delta(E - \epsilon(k)) \frac{\pi \hbar}{L} |v_x(k)|$$

⇒ For 1D material.

$$M(E) = \sum_{k_y} \int_{-\infty}^{\infty} \frac{dk_x L}{2\pi} \delta(E - \epsilon(k)) \frac{\pi \hbar}{L} |v_x|$$

$$\text{Now } v_x = \frac{1}{\hbar} \frac{\partial E}{\partial k_x}$$

$$M(E) = \sum_{k_{yn}} \int_{-\infty}^{\infty} \frac{dk_x k}{2\pi} \delta(E - \epsilon(k)) \cdot \frac{\pi \hbar}{k} \cdot \frac{1}{\hbar} \frac{\partial E(k_x)}{\partial k_x}$$

$$n = \underline{\underline{1, 2, 3, \dots}}$$

$$M(E) = \sum_{k_{yn}} \int_{-\infty}^{\infty} \frac{dk_x}{2} \delta(E - \epsilon(k)) \frac{\partial E(k_x)}{\partial k_x}$$

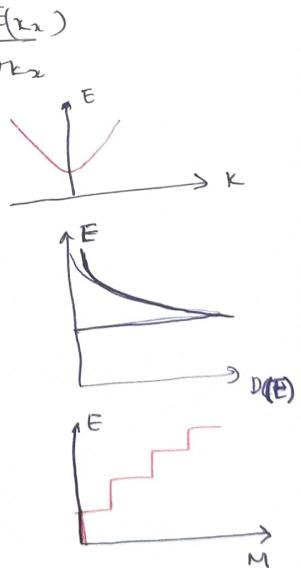
$$M(E) = \sum_{k_{yn}} \frac{1}{2} \int_{-\infty}^{\infty} \delta(E - \epsilon(k)) \cdot dE$$

1st step + 1st step ... n steps

Step 1<sup>st</sup>

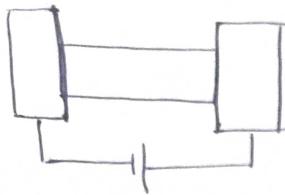
$$M(E) = \textcircled{H} (E - \epsilon(k))$$

$$\text{HW :- } \epsilon(k) = \frac{\hbar^2 k^2}{2m}. \text{ Calculate } D(E) \text{ & } M(E) \rightarrow \text{for 1D, 2D & 3D solids.}$$



# Principles of Quantum Devices

class 20



$$I = \frac{\alpha}{h} \int dE D(E) \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} [f_1 - f_2]$$

if  $\gamma_1 = \gamma_2 = \gamma$

$$I = \frac{\alpha}{h} \int dE D(E) \frac{\gamma}{2} [f_1 - f_2] = \frac{\alpha}{h} \int dE \underbrace{[\gamma D(E) \gamma]}_{M(E)} [f_1 - f_2]$$

$$\Rightarrow I = \frac{\alpha}{h} \int dE M(E) [f_1 - f_2]$$

We know  $D(E) = \sum \delta(E - E(k))$

$$M(E) = \pi D(E) \gamma$$

$$\gamma = \frac{\hbar v_x}{L}$$

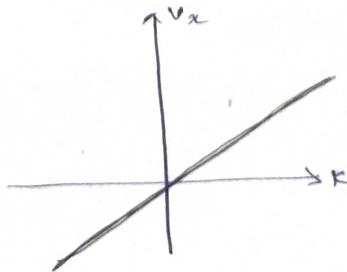
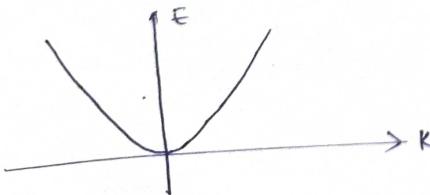
$$M(E) = \sum \delta(E - E(k)) \pi \frac{\hbar v_x}{L}$$

$$v_x = \frac{1}{\pi} \frac{dE}{dk}$$

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

$$v_x = \frac{1}{\pi} \frac{\hbar^2 k}{m} = \frac{1}{m} \cdot \frac{\hbar k}{\pi}$$

$$\Rightarrow v_x = \sqrt{\frac{2E}{m}}$$



How to find  $D(E)$  from  $E-k$ ?

For 1D

$$D(E) = \int_{-\infty}^{\infty} \frac{dk}{2\pi/L} \delta(E-E) = 2 \int_0^{\infty} \frac{L}{2\pi} dk \delta(E-E)$$

have to convert to  $\frac{dk}{E}$   
from  $E-k$  relation.

$$D(E) = \frac{L}{\pi} \int_0^{\infty} dE \left( \frac{dk}{dE} \right) \cdot \delta(E-E)$$

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

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

$$\left\{ \frac{dk}{dE} = \frac{m}{\hbar^2 k} \right\}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{1}{\hbar} \sqrt{2mE}$$

$$\frac{dk}{dE} = \frac{m}{\hbar \sqrt{2mE}} \quad \nu_2 = \frac{1}{\pi} \frac{dE}{dk}$$

$$D(E) = \frac{L}{\pi} \int_0^{\infty} dE \frac{m}{\hbar \sqrt{2mE}} \cdot \delta(E-E)$$

$$\left( \frac{L}{\pi} \frac{dE}{dE} \right) = \frac{L}{\pi \hbar \sqrt{2mE}}$$

$$D(E) = \frac{L}{\pi} \cdot \frac{m}{\hbar \sqrt{2mE}} = (\cdot) E^{-1/2}$$

using similar process, if we find  $D(E)$ ,  $MCE$ )

	$D(E)$	$MCE$ )
1D	$\sim \sqrt{E}$	$\sim E^0$
2D	$\sim E^0$	$\sim E^{1/2}$
3D	$\sim \sqrt{E}$	$\sim E$

For a 2 dimensional solid

$$w \quad L$$
$$S = w \cdot L$$

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

$$D(E) = \frac{m}{2\pi\hbar^2}$$

$$N = \int dE D(E) \cdot f_0(E)$$

@ T=0K  
 $f_0(E) = \mu$   
 $f_0(E) \rightarrow \text{chemical potential}$

$$N = \int dE \cdot \frac{m}{2\pi\hbar^2} \cdot \mu = \frac{m}{2\pi\hbar^2} \mu \cdot S.$$

$\approx 2$  factor coming due to spin  
(No. of es per unit area)

$$\frac{N}{S} = n_s = \frac{m}{\pi\hbar^2} \cdot \mu$$

$$n(E) = \sqrt{\frac{2mE}{\hbar}} \cdot \frac{w}{\pi}$$

$$I = \frac{2\alpha}{\hbar} \int dE M(E) (f_1 - f_2)$$

$$\Rightarrow I = \frac{2\alpha}{\hbar} \mu(u) \int_{\alpha/\sqrt{v}}^{dE} (f_1 - f_2) = \frac{2\alpha^2}{\hbar} M(u) \sqrt{v}$$

$$\Rightarrow g = \frac{I}{\sqrt{v}} = \frac{2\alpha^2}{\hbar} \cdot \frac{w}{\pi\hbar} \sqrt{2m\mu}$$

$$\Rightarrow R = \frac{\pi\hbar w}{w \cdot 2\alpha^2} \cdot \frac{1}{\sqrt{2m\mu}}$$

$$\Rightarrow RW = \pi\hbar \cdot \frac{w}{2\alpha^2} \cdot \frac{1}{\sqrt{2m\mu}} = \cancel{n} \cdot \frac{w}{2\alpha^2} \sqrt{\frac{\pi^2 k^2}{2 \cdot \pi \hbar^2 m \mu}}$$

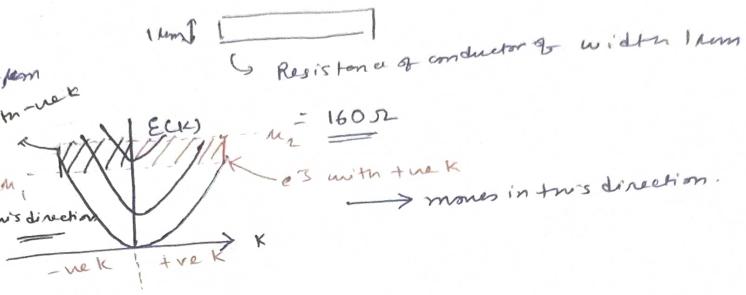
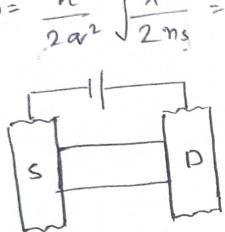
$$\therefore RW = \frac{w}{2\alpha^2} \sqrt{\frac{\pi}{2m\mu}} = 160 \text{ nm}$$

$n_s = \frac{m\mu}{\pi\hbar^2}$   $\Rightarrow m\mu = n_s \cdot \pi\hbar^2$

$10^{12} / \text{cm}^{-2}$

$$I = \frac{2\alpha}{h} \int dE M(E) (f_1 - f_2)$$

$$R_W = \frac{n}{2\alpha^2} \sqrt{\frac{\pi}{2m}} = 160 \Omega/\text{mm}$$



So, some  $e^-$ s are moving in L-R, some from R-L.

What happens if there are scatterers in the channel?

→ The current expression has to be updated, as the scatterers change the amount of current flowing (due to scattering.)

Let's say if  $100 e^-$ s are transferred in the channel,  $80 e^-$ s will pass through, but  $20 e^-$ s will be reflected back after scattering.

$\therefore R + T = 1$

Ratio of transmitted  $e^-$ s.

Ratio of reflected  $e^-$ s.

∴ The current will be dependent on  $T$ , which is the factor of  $e^-$ s which are transmitted through the channel.

The electrons are getting reflected or not, is a function of the Energy of the electron.

Hence the factor of transmitted electron (CT) is a function of Energy as well.  $\therefore T(E)$

For application of small voltages

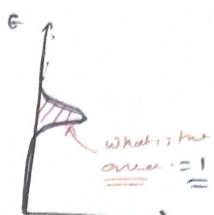
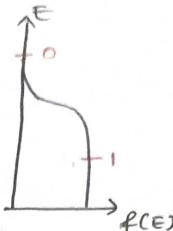
$$I = \frac{2\alpha}{h} \int dE M(E) \left( -\frac{\partial f}{\partial E} \right) \alpha V \underset{T(E)}{=}$$

Transmitted  $e^-$  factor

$$G_T = \frac{I}{V} = \frac{2\alpha^2}{h} \int dE M(E) \left( -\frac{\partial f}{\partial E} \right) T(E)$$

$$\Rightarrow G_T = \frac{2\alpha^2}{h} M.T.$$

value of M.T. averaged over  
 $\int \frac{df}{dE}$



$$\frac{\partial f}{\partial E}$$

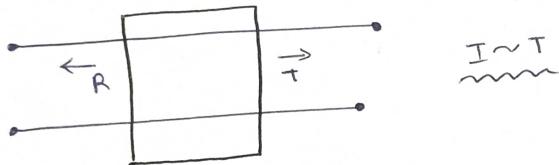
Landauer formula:-

$$\text{where } M.T. = \int dE \left( -\frac{\partial f}{\partial E} \right) M(E) T(E)$$

for a single mode  $M(E) = 1$

$M(E) \rightarrow \underline{\text{mode}}$ . For this case, we are basically averaging over T.

$$\int dE \left( \frac{\partial f}{\partial E} \right) = \int_0^1 Sf = 1$$



$$\text{As } G_T = \frac{2\alpha^2}{h} M.T \quad \therefore R = \frac{1}{\alpha} = \frac{n}{2\alpha^2} \cdot \frac{1}{M} \cdot \frac{1}{T} \xrightarrow{\substack{R + R_{\text{contact}} \\ (\text{Scattering + Contact resistance})}}$$

(Presence of scatterers adds resistance to the channel.)

$R \rightarrow \underline{\text{Reflection}}$

$$\text{Landauer Resistance : } R = \frac{h}{2\alpha^2 M} \frac{1}{T} R$$

$$\Rightarrow R_S = \frac{n}{2\alpha^2 M} \frac{1-T}{T} R \quad \begin{matrix} \text{(Landauer calculated using} \\ \text{this formula)} \end{matrix}$$

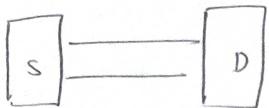
The two formulae are different.. (The first one does not have any  $\underline{\text{L.T.}}$ )

If we add the term  $\left( \frac{n}{2\alpha^2} \cdot \frac{1}{M} \right)$  with Landauer resistance,

$$R_S = \frac{n}{2\alpha^2 M} \frac{1-(1-T)}{T} + \frac{n}{2\alpha^2} \cdot \frac{1}{M} = \frac{n}{2\alpha^2} \cdot \frac{1}{M} \left( \frac{1}{T} - 1 + T \right)$$

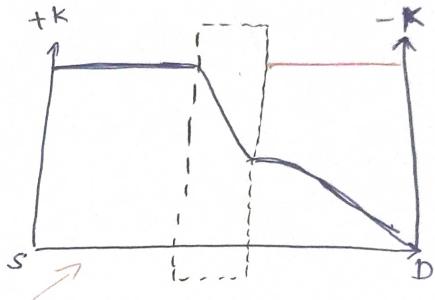
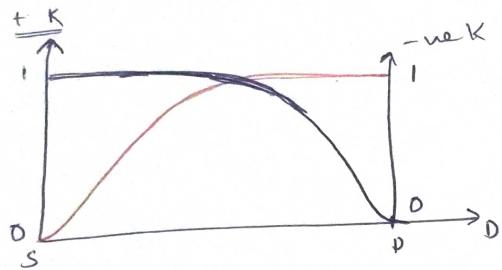
$$\begin{matrix} \uparrow \\ \text{Scattering} \\ \text{Contact} \\ \text{resistance} \end{matrix} = \frac{n}{2\alpha^2} \cdot \frac{1}{MT}$$

How does the K of electrons change in a channel.



At the source, all the  $e^-$ 's are moving towards the the K direction, and no  $e^-$ 's in the -ve K direction.

At the drain, all  $e^-$ 's move in -ve K direction, and no  $e^-$ 's move in the +ve K direction.

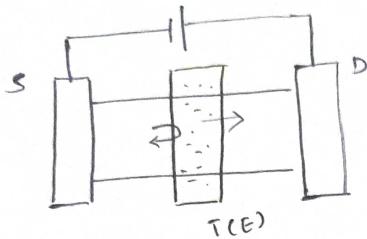


If there is a scattering region in the channel.

# Principles of Quantum Devices

class - 22  
Date - 2023

## Landauer Formula



$$I = \frac{2eV}{h} \int dE M(E) T(E) [f_1 - f_2]$$

$$\Rightarrow G_L = \frac{I}{V} = \frac{2e^2}{h} \int dE M(E) T(E) \left( \frac{-\partial f}{\partial E} \right)$$

$$\Rightarrow G_L \approx \frac{2e^2}{h} \frac{MT}{T}$$

Basically like averaging  
M(E) over T(E) for a  
specific noise.

$$\tilde{M}T = \int dE \left( -\frac{\partial f}{\partial E} \right) M(E) T(E)$$

$$R = \frac{n}{2e^2} \cdot \frac{1}{M} \cdot \frac{1}{T} \quad | \text{ has both channel & contact resistances}$$

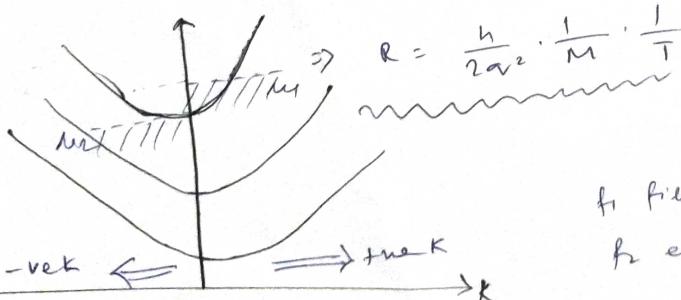
Original Landauer formula: -  
(Does not consider the contact resistances)

To connect the Landauer formula, we have to add the contact resistance to it.

$$\therefore R = \frac{n}{2e^2} \cdot \frac{1}{M} \cdot \frac{1-T}{T} + \frac{h}{2e^2} \cdot \frac{1}{M}$$

contact resistance

$$\Rightarrow R = \frac{n}{2e^2} \cdot \frac{1}{M} \left( \frac{1}{T} - 1 \right) + \frac{h}{2e^2} \cdot \frac{1}{M}$$

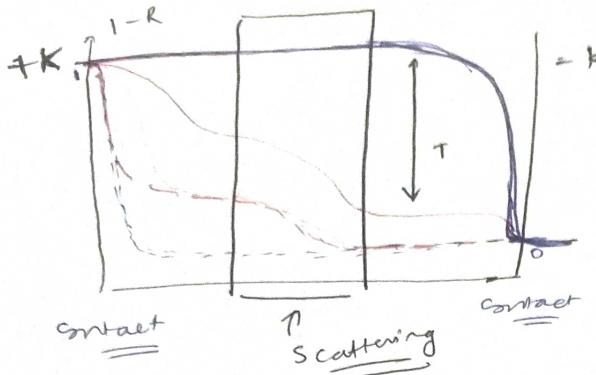


$f_1$  fills up the K e's

$f_2$  empties the K e's

$$\therefore I \propto (f_1 - f_2)$$

But what happens if there are scatterers? (not all e's injected comes out)



no scattering  
 --- - vek  
 ——— true K.  
  
With scattering  
 --- - vek K  
 ——— true K

$$T = \frac{\lambda}{\lambda + L}$$

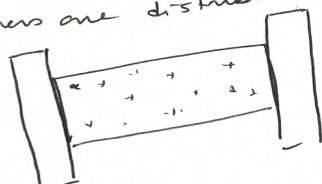
$\Rightarrow$  Mean free path  
 $\hookrightarrow$  Distance (Device length).

when  $\lambda \gg L$  :  $T \rightarrow 0$  (Ballistic Transport)

$$\frac{x \ll L}{=} \quad T = \frac{\rho}{L}$$

$\gg L$   $T = \frac{\partial}{\partial z}$   
 If scatterers are distributed uniformly across the channel,  
 $I = I_+ - I_-$

$$I = I^+ - \underline{I^-}$$



A circuit diagram illustrating node analysis. Two nodes are shown: node  $K$  at the top and node  $-K$  at the bottom. A horizontal line connects these two nodes. A red arrow labeled  $I_1$  enters node  $K$  from the left. A red arrow labeled  $I_2$  leaves node  $K$  towards the right. Between the two nodes, there is a vertical line with a double-headed arrow labeled  $dI/dx$ , representing a voltage source. To the left of node  $K$ , there is a label  $= +K$ . To the right of node  $-K$ , there is a label  $+K \} I \text{ (constant)}$ . Below node  $-K$ , there is a label  $I_2^- = 0$ .

$$\frac{dI^+}{dt} = (-I^+ + I^-) \frac{dL}{\partial}$$

current at  $d x$ ?

$$\frac{dI^+}{dx} = -\frac{I^+}{R}$$

$$\frac{dI^+}{dx} = \frac{I^+}{\lambda} \Rightarrow I^+ = \frac{I^+}{\lambda} x + C$$

$$\frac{dI^+}{dx} = - \frac{I^-}{\lambda} = \frac{dI^-}{dx}$$

unknown  
 $I^+ = \alpha n^{+v}$        $I^- = \alpha n^{-v}$

$$\frac{dI^+}{dx} + \frac{dI^-}{dx} = - \frac{2I}{\lambda}$$

$$\Rightarrow \frac{d}{dx} \{ I^+ + I^- \} = - \frac{2I}{\lambda}$$

$$\Rightarrow \alpha v \frac{dn}{dx} = - \frac{2I}{\lambda}$$

$$\Rightarrow I = - \alpha \left( \frac{v \lambda}{2} \right) \frac{dn}{dx} = - \alpha D \frac{dn}{dx}$$

↓  
diffusion coefficient