

Intro to

Semiconductors

Time Independent SE in 1-D:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + U(x) \psi_E(x) = E \psi_E(x)$$

$\psi_E$  is energy eigen state with energy  $E$

$U(x)$  is potential energy

Free Particles:  $U(x) = 0$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_E(x)}{dx^2} = E \psi_E(x)$$

$$\psi_E(x) = e^{ikx}$$

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

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

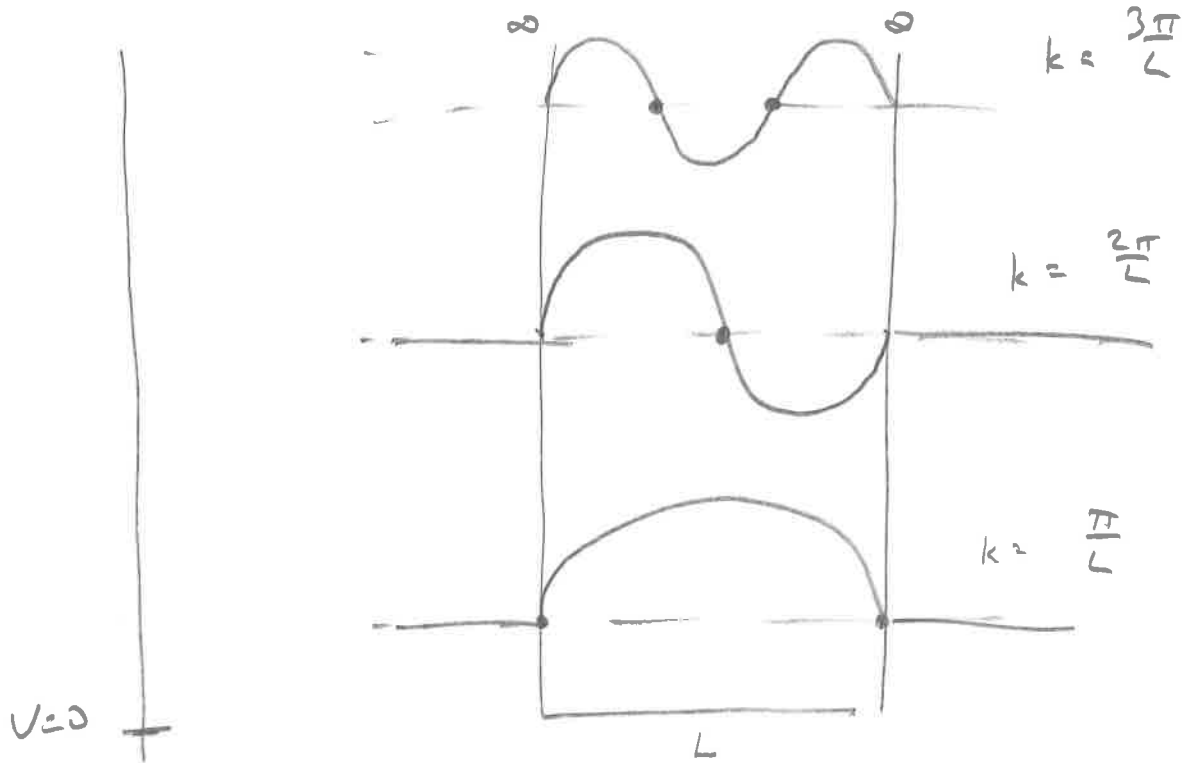
$$\boxed{p = \hbar k}$$

$\psi_E \sim e^{ikx}$  is free particle with

momentum  $p = \hbar k$ ,  $k$  is a continuous

variable (no quantization).

# Particle In Infinite Well



Wave equation must go to zero at boundary.

Solution inside is free-particle.

Energy can be calculated because in well,  $U(x) = 0$  and

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

\*\*\* More nodes = higher energy ! \*\*\*

## General Sketching of Wave Equations

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_E(x) = [E - U(x)] \psi_E(x)$$

### Qualitatively

- 1)  $\psi_E$  is continuous everywhere, and goes to 0 as  $x \rightarrow \pm \infty$
- 2) Where  $E > U(x) \rightarrow$  oscillatory function
- 3) Where  $E < U(x) \rightarrow$  exponential
- 4)  $E \sim \# \text{ nodes}$
- 5)  $\psi_E$  has no kinks if potentials are finite

Proof (5):

RHS looks at  $\frac{d^2 \psi}{dx^2}$



$$= \frac{d^2 \psi}{dx^2}$$

$$\Rightarrow \frac{d\psi}{dx} =$$



$\leftarrow$  kink

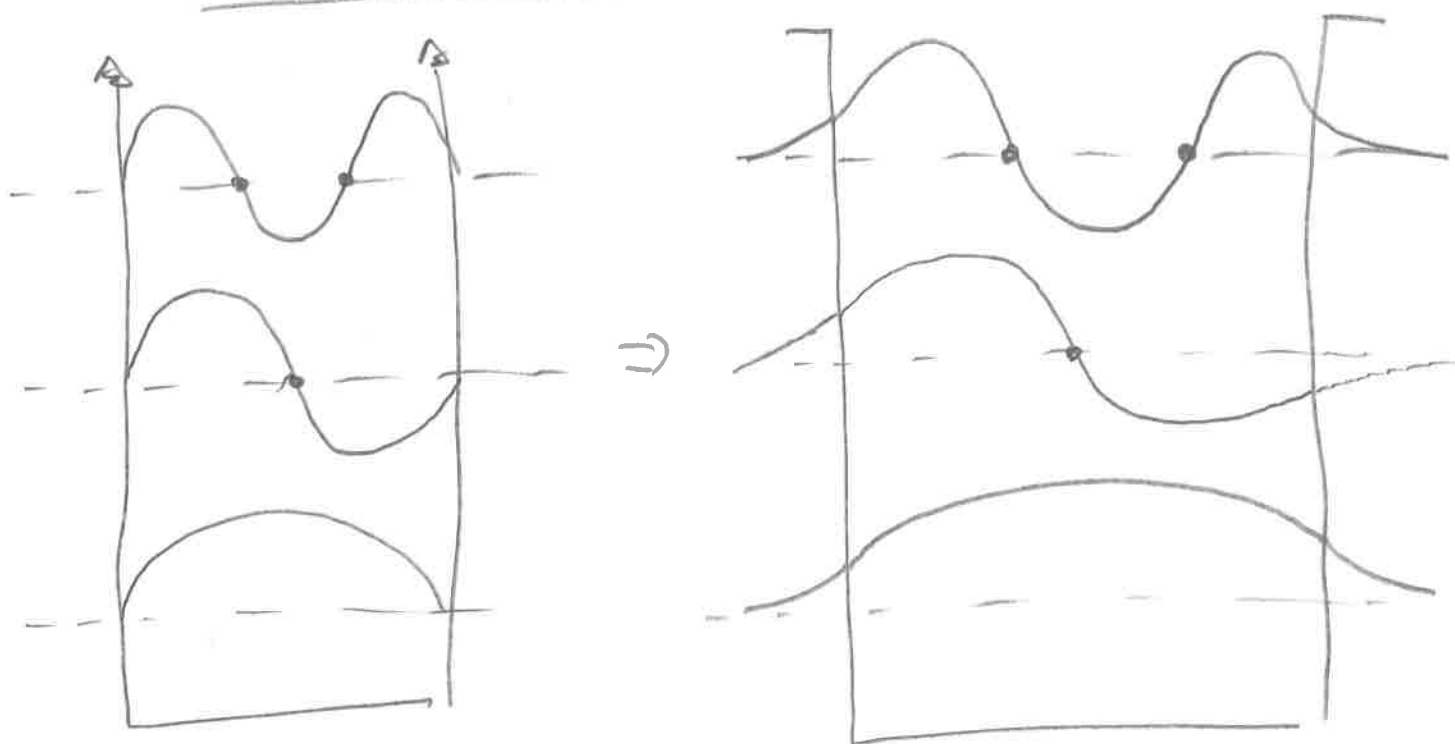
$\psi$

$\rightarrow$

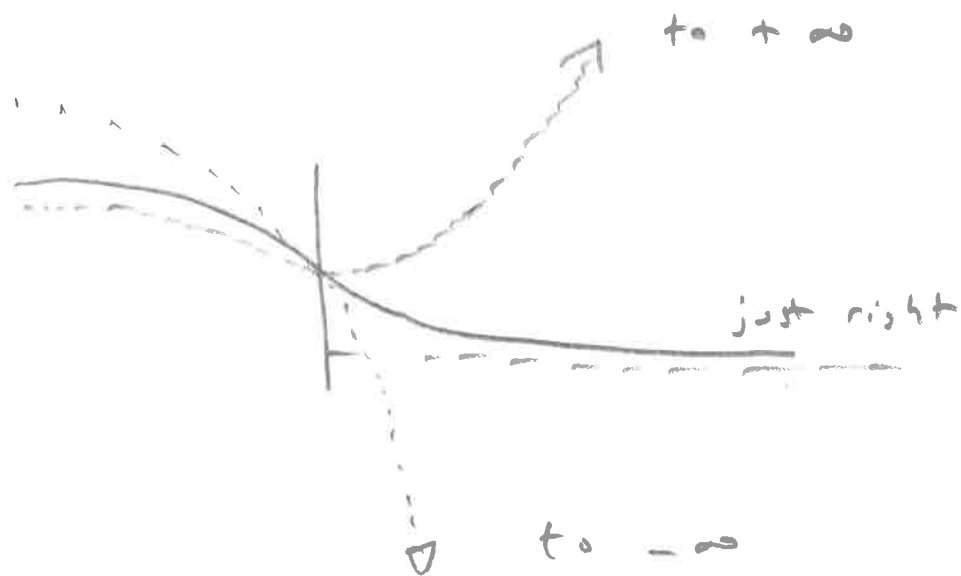


$\leftarrow$  smooth

## Particles in Finite Well

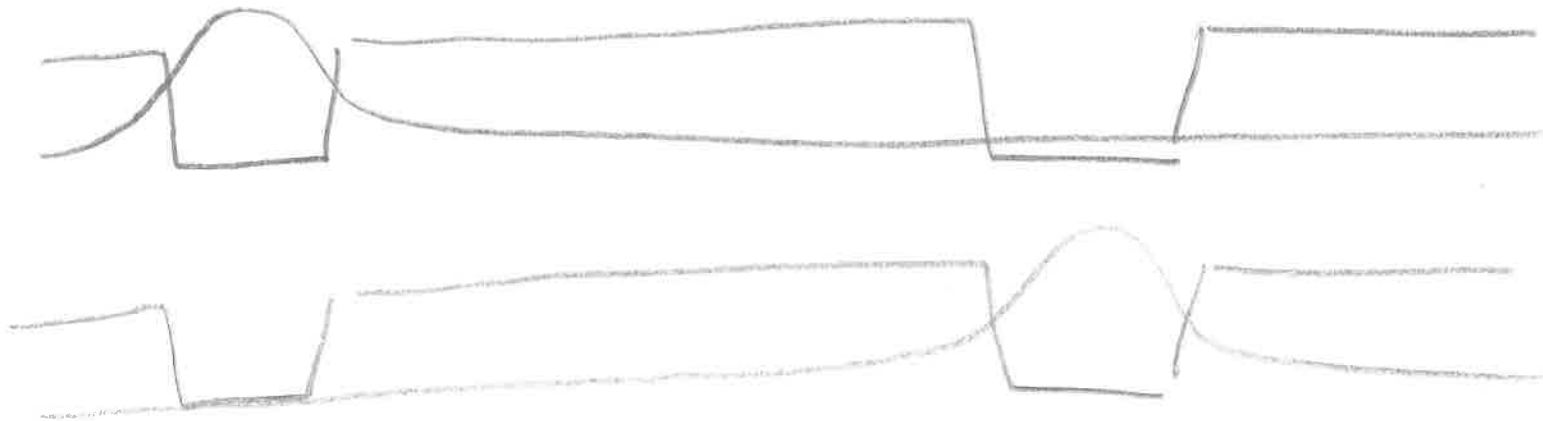


Quantization persists because only certain values of  $E$  tie an oscillatory solution to an exponential that doesn't diverge as  $x \rightarrow \infty$

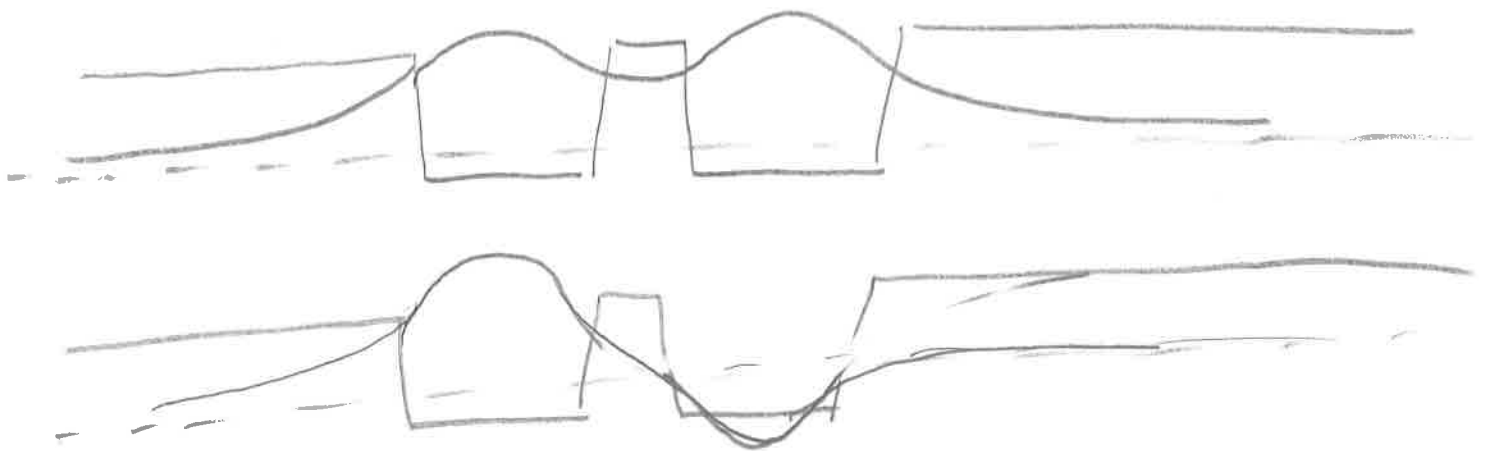


Two particles in two wells:

Far Apart



But close together



Must be even or odd, due to symmetry.  
Odd solution (asymmetric) has higher  
energy, due to one more node.

$$\begin{array}{c}
 \uparrow \\
 \frac{n=2}{\quad} < \frac{\frac{k=2}{k=1}}{\quad} \quad n=2 \\
 \\
 \frac{n=1}{\quad} < \frac{\frac{k=2}{k=1}}{\quad} \quad n=1
 \end{array}$$

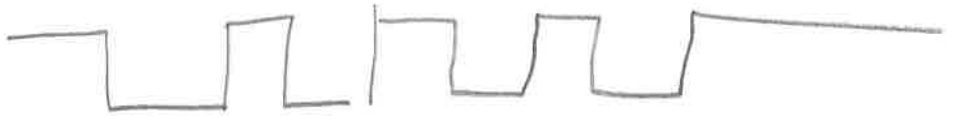
Chemistry



(Energy of covalent bond is  $2 \Delta E \dots$ )

"This is, like, 70% of chemistry"  
goes over well!

4 wells



"Envelope"



0 nodes



1 node



2 nodes



3 nodes



$n = 2$

—



$n = 1$

—





For periodic rotation



Block showed

$$\psi(x) = e^{ikx} u_k(x)$$

where  $e^{ikx}$

$$u_k(x) = u_k(x+a)$$

$k$  is continuous;

The "envelope" is continuous



Looks like a free particle

with momentum

$$p = \hbar k.$$

$n=2$  \_\_\_\_\_

$$\begin{array}{r} k=4 \\ \hline k=3 \\ \hline k=2 \\ \hline k=1 \end{array}$$



$k$  continuous

$n=1$  \_\_\_\_\_

$$\begin{array}{r} k=4 \\ \hline k=3 \\ \hline k=2 \\ \hline k=1 \end{array}$$



$k$  continuous

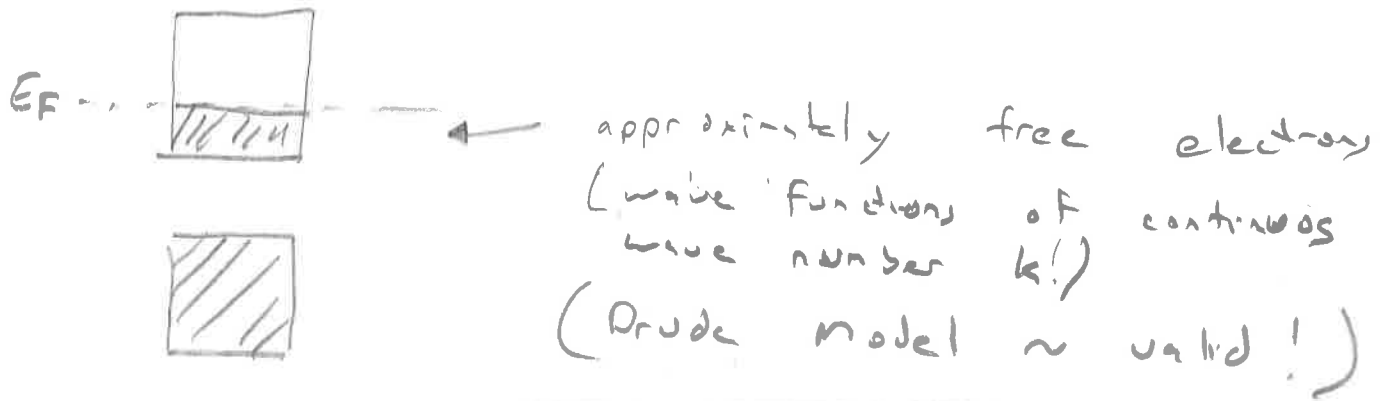
1 atom

4 atoms

$10^{23}$  atoms

\* Within bands, wave equations are similar to free particle wave equations, with continuous value "k".

## Conductors:



Recall:  $\sigma \sim n q^2 \tau / m$

Q: What about a completely full band? Can it conduct?



Answer: No ...




Why?

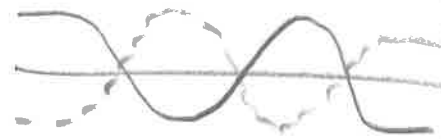
$$\psi_1 = e^{i(kx - \omega t)}$$

R travelling  
→  
Re  $\psi_1$  

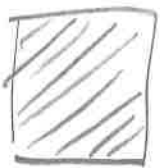
$$\psi_2 = e^{i(-kx - \omega t)}$$

L travelling  
←  
Re  $\psi_2$  

$$\begin{aligned} \psi_1 + \psi_2 &= e^{-i\omega t} \cdot (e^{ikx} + e^{-ikx}) \\ &= e^{-i\omega t} 2 \cos kx \end{aligned}$$



↗  
Standing wave



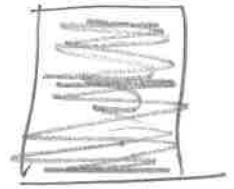
↖ In full Energy band, all  
k-states are full, and  
wave in one direction exactly  
cancelled by wave in  
another direction.

There's no way, with small amount  
of energy, for total wave function  
to have net current...

(End Lecture 1)

# Recap:

$n=2^1$



$n=1$



1 atom



2 atoms

(Origin of bands)



4 atoms



$10^{23}$  atoms

Continuous bands,  
when full, no  
conduction  
possible!

Conduction  
+  
Valence



Conduction



Conduction



Valence

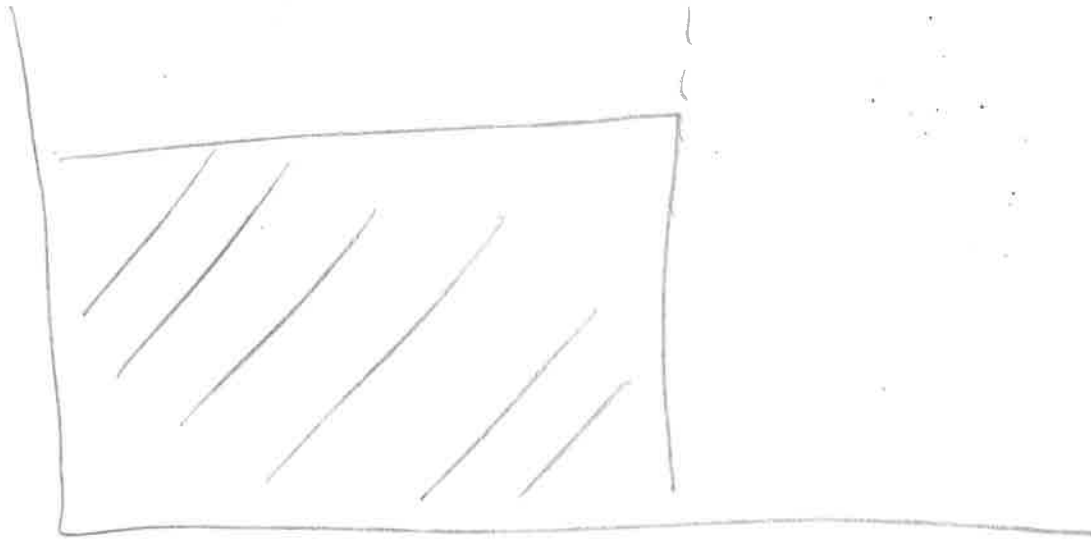
Insulator

Conduction Band = lowest band not fully occupied ( $@T=0$ )  
Valence Band = highest band not empty ( $@T=0$ )

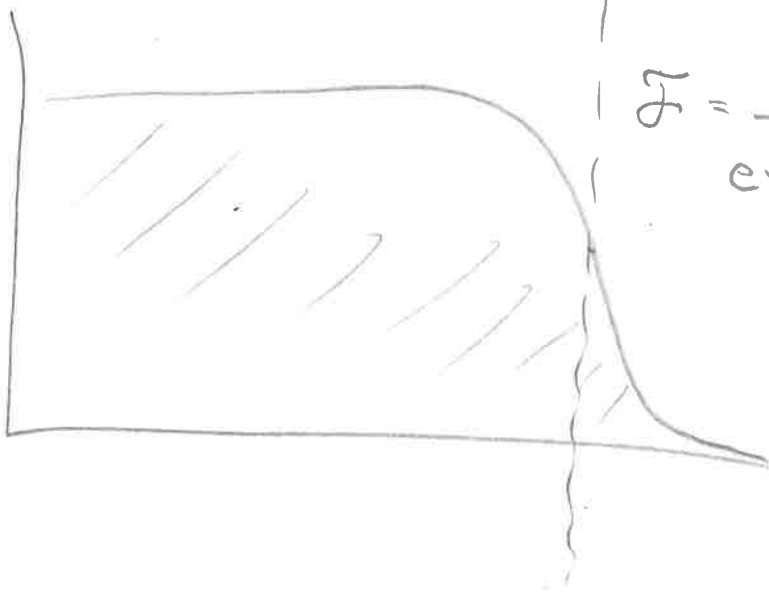
# Fermi - Dirac Distribution

$$T = 0$$

$$E_F$$



$$T > 0$$



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

$E$

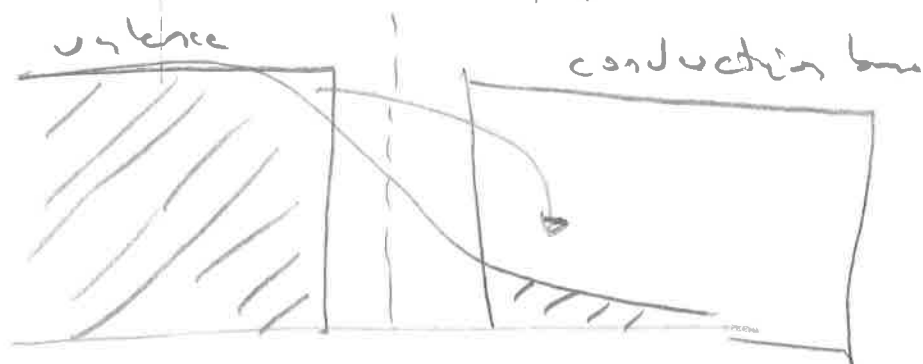
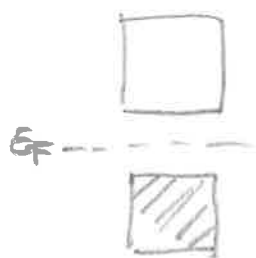
At  $E \gg E_F$

$$f \sim \exp\left(-\frac{E - E_F}{kT}\right)$$

which looks like a boltzmann factor  
but relative to the  $E_F$ .

Intrinsic Semiconductors:

$T > 0$



$E_F$  is midway, equal number of electrons in conduction band, and vacant electron states in valence band (holes).

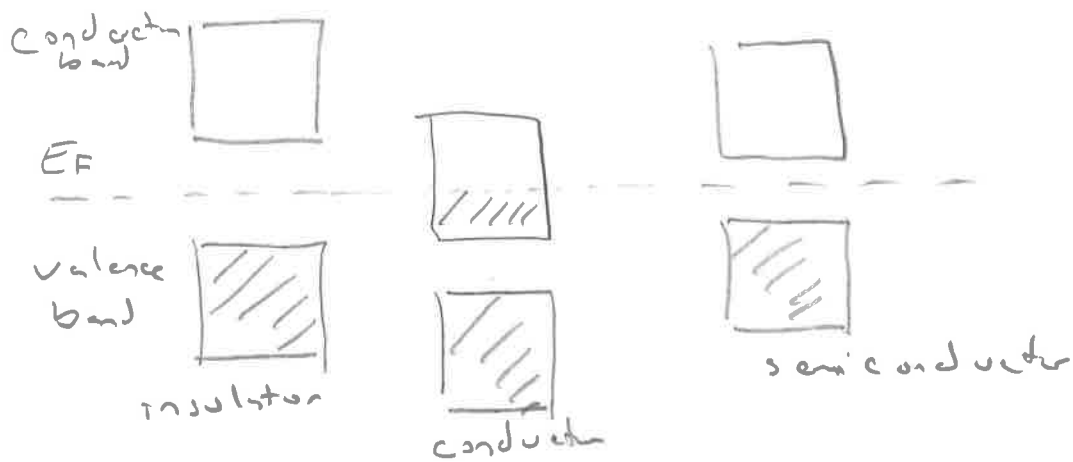
Holes are mobile charge carriers as well as electrons in valence band, \*



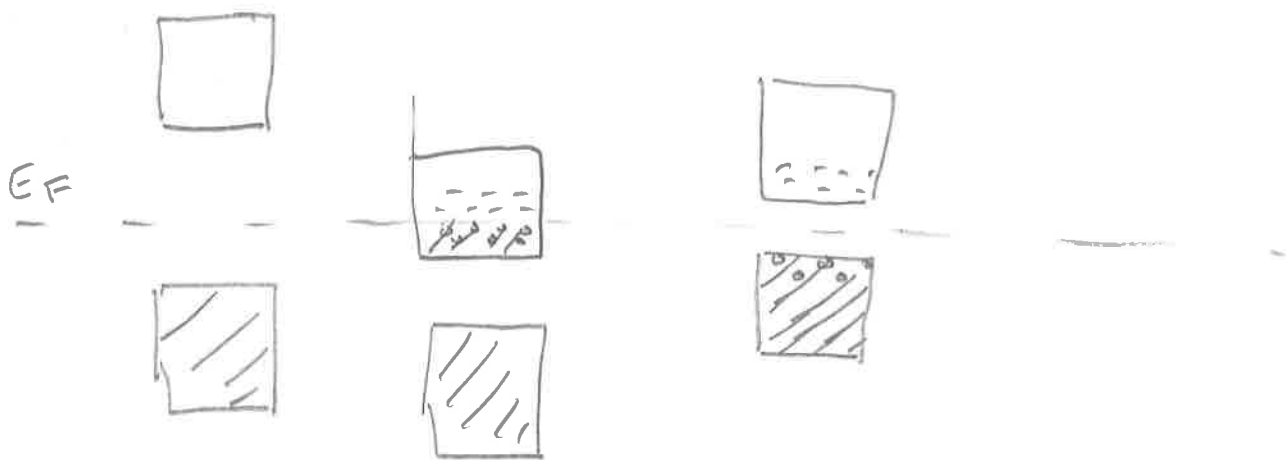
Intrinsic semiconductors have equal #'s :  $p = n$

(\*) More accurately think of standing wave  $\psi_L + \psi_R$  minus one component  $\psi_L$  ...

$$T = 0$$



$$T \sim 275 \text{ K}$$



Semiconductors have small band gap ( $\sim 1 \text{ eV}$ ) such that thermal fluctuations lead to electrons in conduction band (and holes in valence band)



Exercise: Given that band gap is  $\sim 1\text{eV}$ , estimate how much less conductive semiconductors are compared to conductors.

Soln:

Recall  $\sigma = \frac{n q^2 \tau}{m}$

Assume  $\tau$  is comparable and only difference in  $\sigma$  is from  $n$ , density of mobile charge carriers (which will assume we just electrons in conduction band)

$$\frac{\sigma_{sc}}{\sigma_c} = \frac{n_{sc}}{n_c} = \exp\left(-\frac{E - E_F}{kT}\right)$$

$$= \exp\left(-\frac{E_g/2}{kT}\right)$$

$$E_g = 1\text{eV} \quad kT \text{ at } 275 \sim \frac{1}{40} \text{eV}$$

$$\frac{\sigma_{sc}}{\sigma_c} = \exp(-40/2) = \exp(-20) = 10^{-9}$$

$\sigma(Cu) = 10^7 \text{ S/m}$   
 $\sigma(Si) = 10^{-3} \text{ S/m}$

## (Next For Lecture)

Aside: why is  $E_F$  defined at midway

between highest occupied and lowest unoccupied? (Or, why is such a gap the chemical potential?)

Ans:  $E_F$  is the "chemical potential" for the fermions, i.e. the energy at which it is at equilibrium,  
So consider



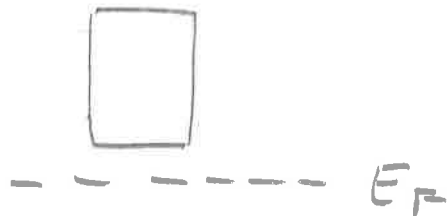
$S1$  is not in equilibrium with  $S2$ , since  $S1$  can donate to  $S2$  for  $\Delta U_{TOT} < 0$ .  
But  $S2$  can donate to  $S1$  only at  $\Delta U_{TOT} = E_G$ .

$S1$  and  $S3$  are in equilibrium,

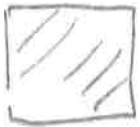
$S1 \rightarrow S3$  cost  $E_G/2$

$S3 \rightarrow S1$  costs  $E_G/2$  !

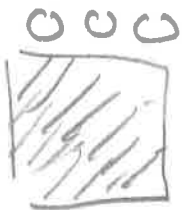
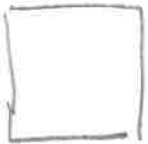
By doping semiconductor, artificial electron absorber or donors can be placed near valence or conduction bands



\* shifts  $E_F$   
near conductor

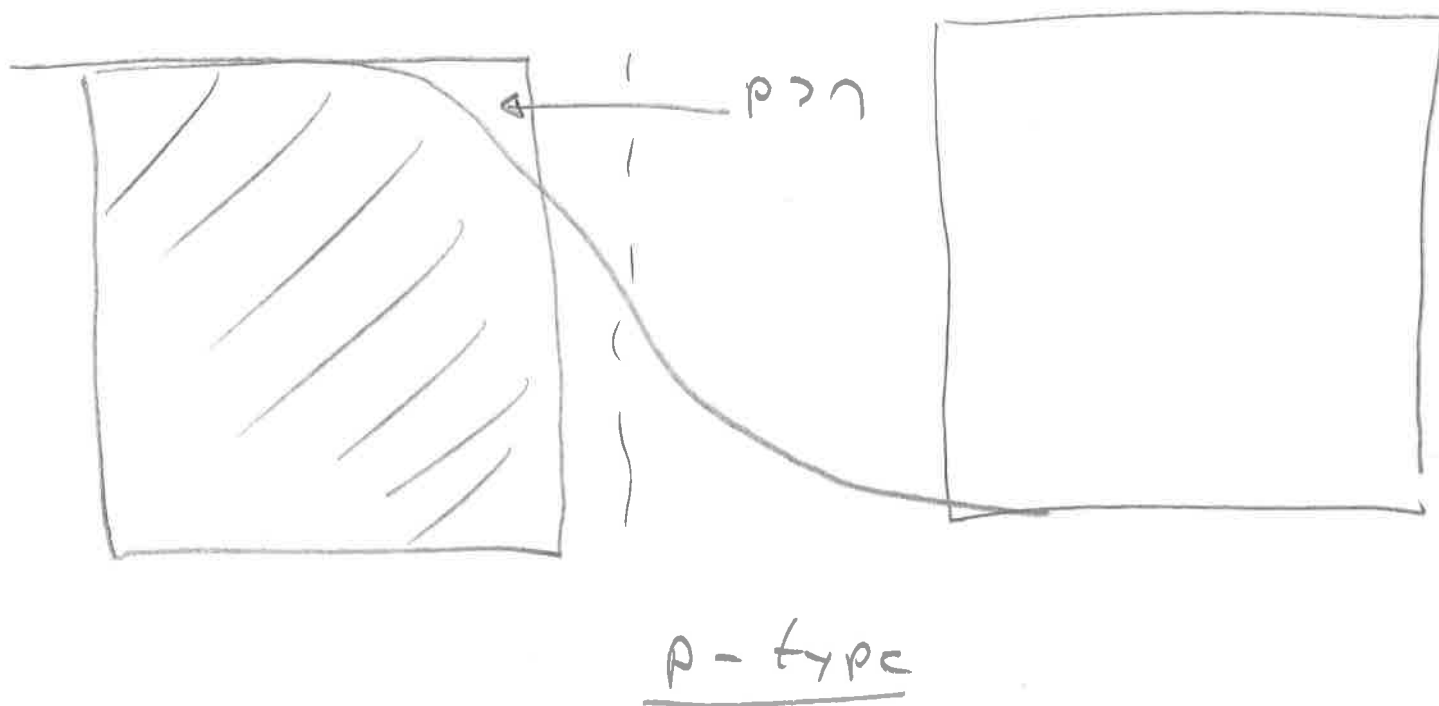
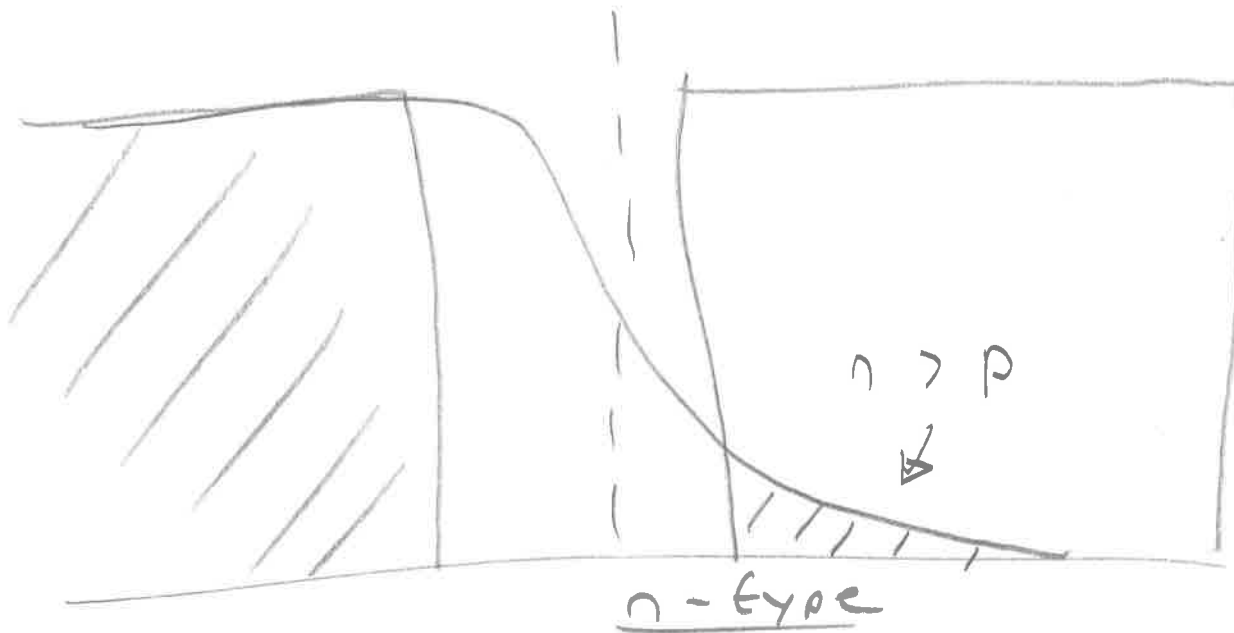


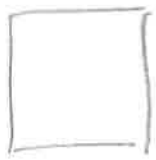
n-type



p-type

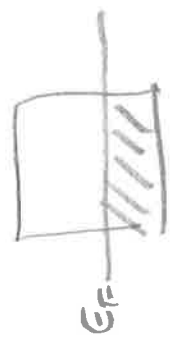
$E_F$



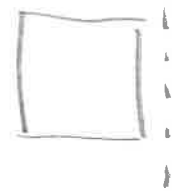


$E_F$  \_\_\_\_\_

Insulators



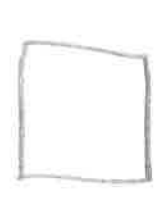
Conductors



intrinsic



n-type



p-type

Semiconductors