

Lecture 1:

Quantum Theory of Solids

- Quantum mechanics
- Free electrons in a box (Fermi gas)
- Band theory of solids
- Fermi/Dirac distribution function
- Doping

Quantum mechanics of free particles:


$$|\Psi(\vec{r}, t)|^2$$

is probability of finding an electron at point r at time t .

Ψ is complex, and both real and imaginary parts are physical.

For a free particle:

$$\Psi(\vec{r}, t) \sim e^{i(\vec{k} \cdot \vec{r} - \omega t)}$$

$$\omega = E / \hbar$$


Momentum:

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

Energy:

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

Schrodinger equation:

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

(1 dimension)

(Time dependent)

Let

$$\Psi(x, t) = A \cdot e^{i(kx - \omega t)}$$

A is a (complex) constant.

Then

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) &= i\hbar \frac{\partial}{\partial t} A \cdot e^{i(kx - \omega t)} = i\hbar(-i\omega) A \cdot e^{i(kx - \omega t)} \\ &= E \cdot A \cdot e^{i(kx - \omega t)} = E \cdot \Psi(x, t) \end{aligned}$$

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t) &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} (A \cdot e^{i(kx - \omega t)}) = \left(-\frac{\hbar^2}{2m} \right) (ik)^2 (A \cdot e^{i(kx - \omega t)}) \\ &= \frac{\hbar^2 k^2}{2m} (A \cdot e^{i(kx - \omega t)}) = \frac{p^2}{2m} \Psi(x, t) \end{aligned}$$

Schrodinger equation: (3 dimensions)

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi(\vec{r}, t)$$

Let $\Psi(\vec{r}, t) = A \cdot e^{i(\vec{k} \cdot \vec{r} - \omega t)} = A \cdot e^{i(k_x \cdot x + k_y \cdot y + k_z \cdot z) - \omega t}$

Then $i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = i\hbar(-i\omega)\Psi(\vec{r}, t) = E \cdot \Psi(\vec{r}, t)$ as before.

But:

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \left(A \cdot e^{i(\vec{k} \cdot \vec{r} - \omega t)} \right)$$
$$= \left(-\frac{\hbar^2}{2m} \right) \left((ik_x)^2 + (ik_y)^2 + (ik_z)^2 \right) \left(A \cdot e^{i(\vec{k} \cdot \vec{r} - \omega t)} \right) = \left(\frac{\hbar^2 (k_x^2 + k_y^2 + k_z^2)}{2m} \right) \Psi(\vec{r}, t)$$
$$= \frac{\hbar^2 k^2}{2m} \left(A \cdot e^{i(\vec{k} \cdot \vec{r} - \omega t)} \right) = \frac{p^2}{2m} \Psi(\vec{r}, t)$$

Quantum mechanics of free particles:

$$\Psi(\vec{r}, t) \sim e^{i(\vec{k} \cdot \vec{r} - \omega t)}$$

Generally,

$$\Psi(\vec{r}, t) = \sum_n A_n e^{i(k_n x - \omega_n t)} \rightarrow \int dk A(k) e^{i(kx - \omega t)}$$

is also a possibility.

Time-independent Schrodinger equation

$$\Psi(\vec{r}, t) = A \cdot e^{i(\vec{k} \cdot \vec{r} - \omega t)}$$

$$= A \cdot e^{i((k_x \cdot x + k_y \cdot y + k_z \cdot z) - \omega t)} = A \cdot e^{i(k_x \cdot x + k_y \cdot y + k_z \cdot z)} \cdot e^{-i\omega t}$$

Call this $\psi(\vec{r})$

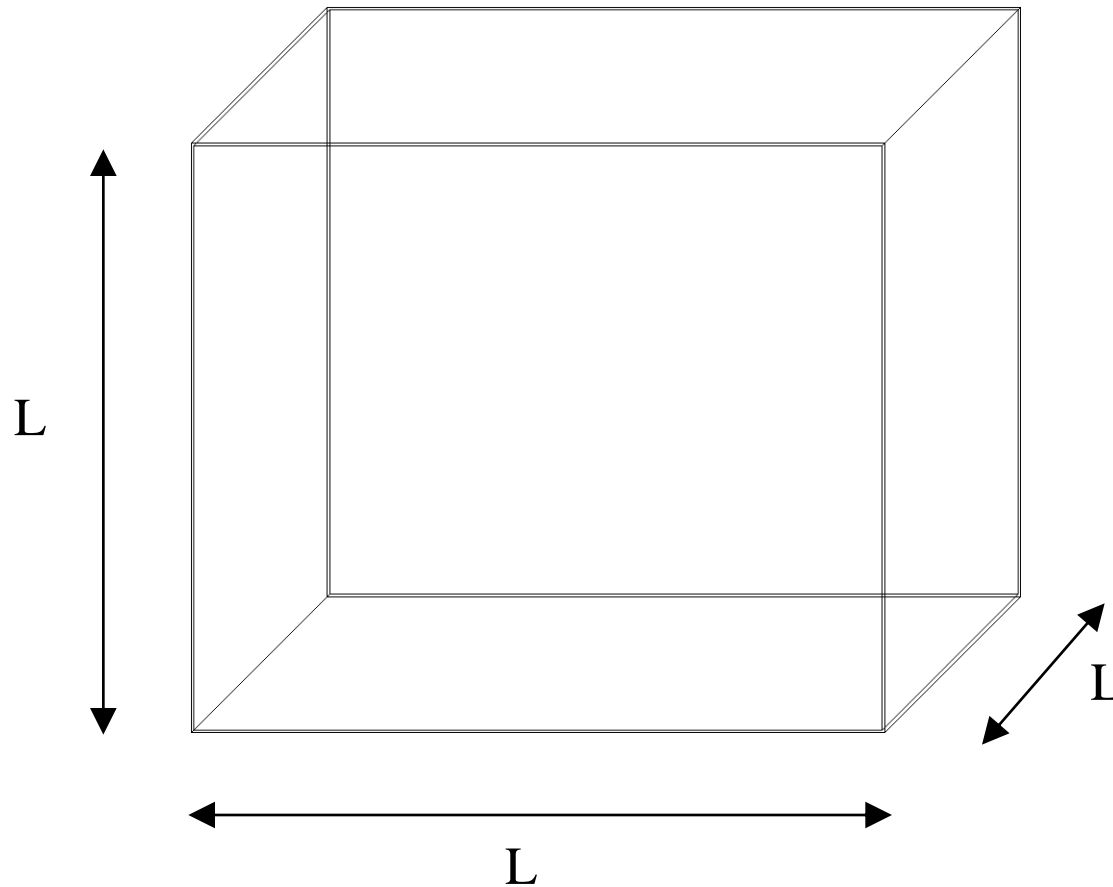
$$\Rightarrow \Psi(\vec{r}, t) = \psi(\vec{r}) \cdot e^{-i\omega t}$$

From:
$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \vec{\nabla}^2 \Psi(\vec{r}, t)$$

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} \psi(\vec{r}) \cdot e^{-i\omega t} = i\hbar(-i\omega)\psi(\vec{r}) \cdot e^{-i\omega t} = E \cdot \psi(\vec{r}) \cdot e^{-i\omega t} = -\frac{\hbar^2}{2m} \vec{\nabla}^2 \Psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi(\vec{r}) \cdot e^{-i\omega t}$$

$$\Rightarrow -\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi(\vec{r}) = E \cdot \psi(\vec{r})$$

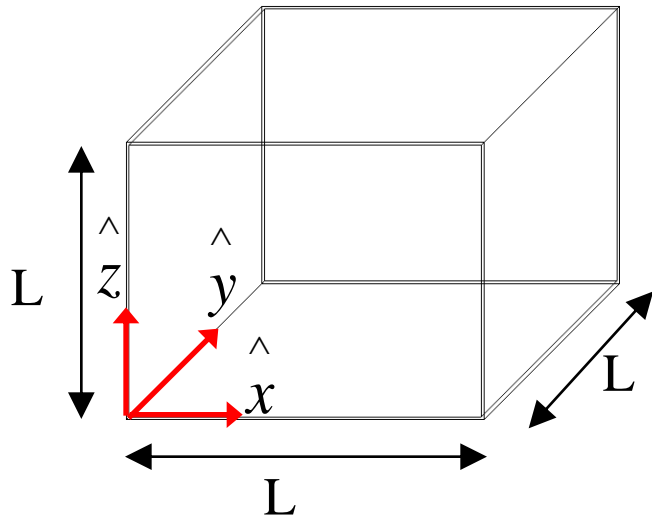
Confined particles: A box



Goal: find $\psi(\vec{r})$

Similar to electric field inside the box.

Goal: find $\psi(\vec{r})$



Everywhere outside the box

$$|\psi(\vec{r})|^2 = 0$$

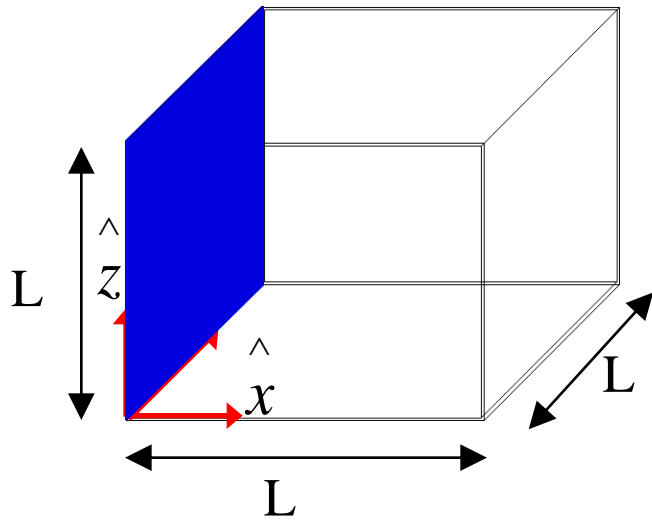
In particular,

$$|\psi(\vec{r})|^2 = 0$$

on the boundaries.

As before, we will consider all six surfaces:

Boundary conditions:



The plane $x=0$:

Try:

$$\psi(\vec{r}) = A \cdot e^{i(k_x \cdot x + k_y \cdot y + k_z \cdot z)}$$

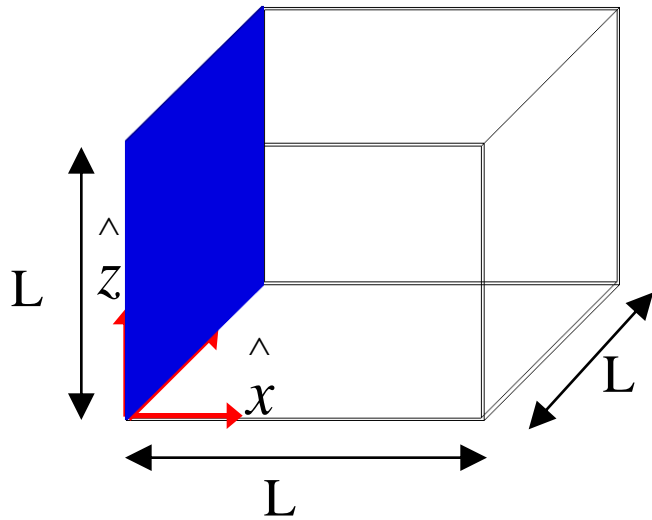
$$\psi(x=0, y, z) = A \cdot e^{i(k_x \cdot \cancel{0} + k_y \cdot y + k_z \cdot z)} = A \cdot e^{i(k_y \cdot y + k_z \cdot z)}$$

Does not solve boundary condition!!!

Boundary conditions: The plane $x=0$:

Let's try something:

$$\psi(\vec{r}) = A \cdot e^{i(k_x \cdot x + k_y \cdot y + k_z \cdot z)}$$



$$-A \cdot e^{i(-k_x \cdot x + k_y \cdot y + k_z \cdot z)}$$

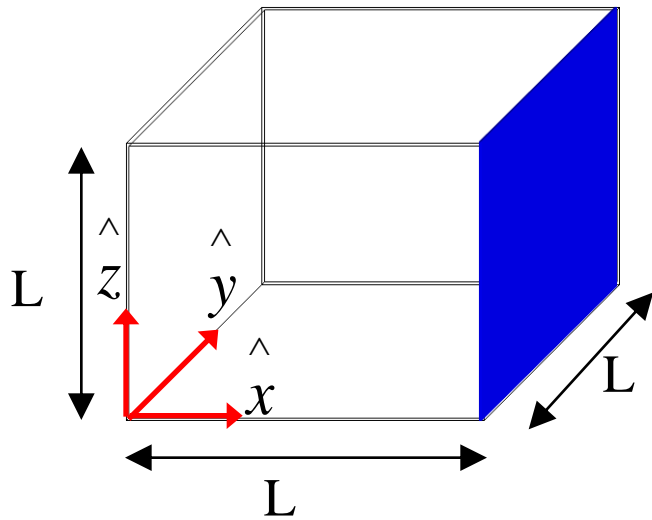
$$\psi(\vec{r}) = A \cdot (e^{ik_x \cdot x} - e^{-ik_x \cdot x}) \cdot e^{i(k_y \cdot y + k_z \cdot z)}$$

$$e^{a \cdot b} = e^a \cdot e^b$$

$$\begin{aligned} \psi(x=0, y, z) &= A \cdot (e^{ik_x \cdot x} - e^{-ik_x \cdot x}) \cdot e^{i(k_y \cdot y + k_z \cdot z)} \\ &= A \cdot (e^0 - e^0) \cdot e^{i(k_y \cdot y + k_z \cdot z)} = 0 \end{aligned}$$

Does solve boundary condition!!!

Boundary conditions: The plane $x=L$:



$$\psi(\vec{r}) = A \cdot \left(e^{ik_x \cdot x} - e^{-ik_x \cdot x} \right) \cdot e^{i(k_y \cdot y + k_z \cdot z)}$$

$$= 2iA \cdot \sin(k_x x) \cdot e^{i(k_y \cdot y + k_z \cdot z)}$$

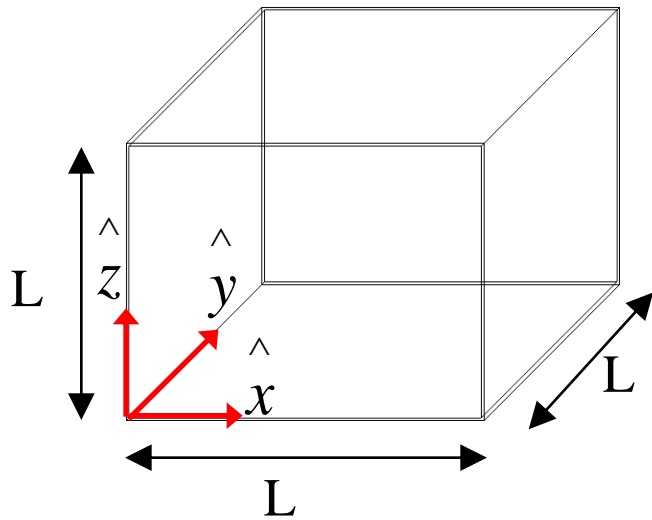
$$\sin(\theta) = \frac{1}{2i} (e^{i\theta} - e^{-i\theta})$$

$$\psi(x = L, y, z) = 2iA \cdot \sin(k_x L) \cdot e^{i(k_y \cdot y + k_z \cdot z)} = 0?$$

If and only if:

$$k_n = n\pi / L$$

Boundary conditions:



We can do the same for y, z:

$$\psi(\vec{r}) = (2i)^3 A \cdot \sin(k_{n_x} x) \cdot \sin(k_{n_y} y) \cdot \sin(k_{n_z} z)$$

$$k_{n_x} = n_x \pi / L$$

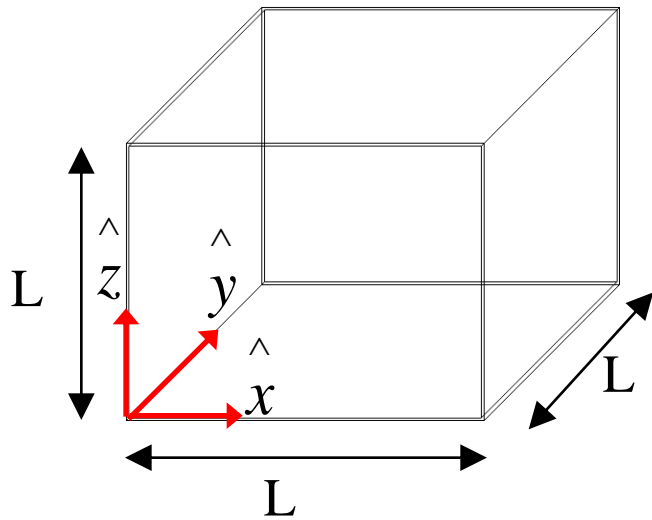
$$k_{n_y} = n_y \pi / L$$

$$k_{n_z} = n_z \pi / L$$

$$E = \frac{\hbar^2 (k_{n_x}^2 + k_{n_y}^2 + k_{n_z}^2)}{2m} = \frac{\hbar^2 (\pi / L)^2}{2m} (n_x^2 + n_y^2 + n_z^2)$$

These are the allowed energy levels, or “quantum states”

Many electrons:

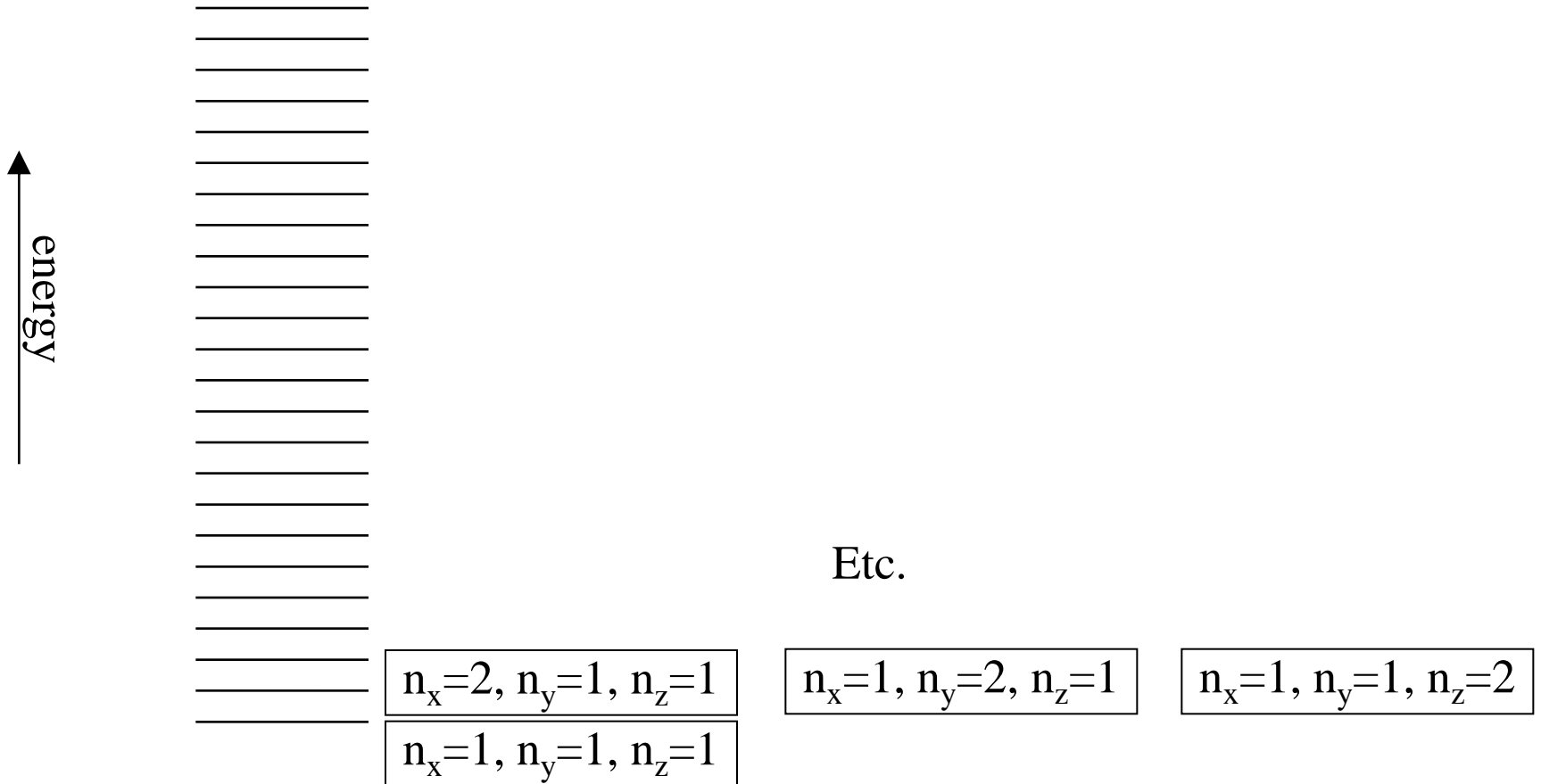


$$E = \frac{\hbar^2 (\pi / L)^2}{2m} (n_x^2 + n_y^2 + n_z^2)$$

These are the allowed energy levels,
or “quantum states”

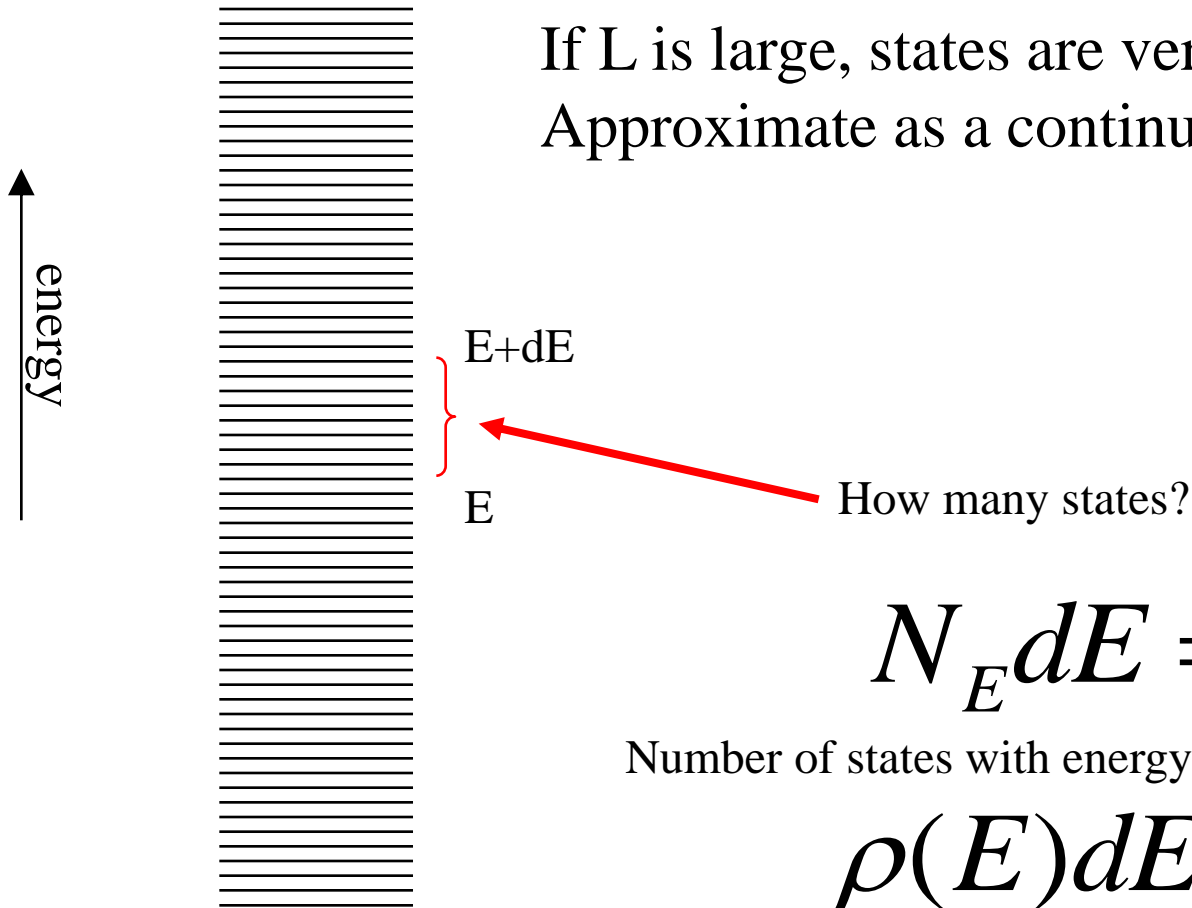
Pauli exclusion principle: Each unique combination of n_x , n_y , n_z can only have two electrons (spin up, spin down).

Energy spectrum of free particles:



Density of states:

If L is large, states are very close together.
Approximate as a continuum.



$$N_E dE = ?$$

Number of states with energy between E and $E + dE$

$$\rho(E) dE = ?$$

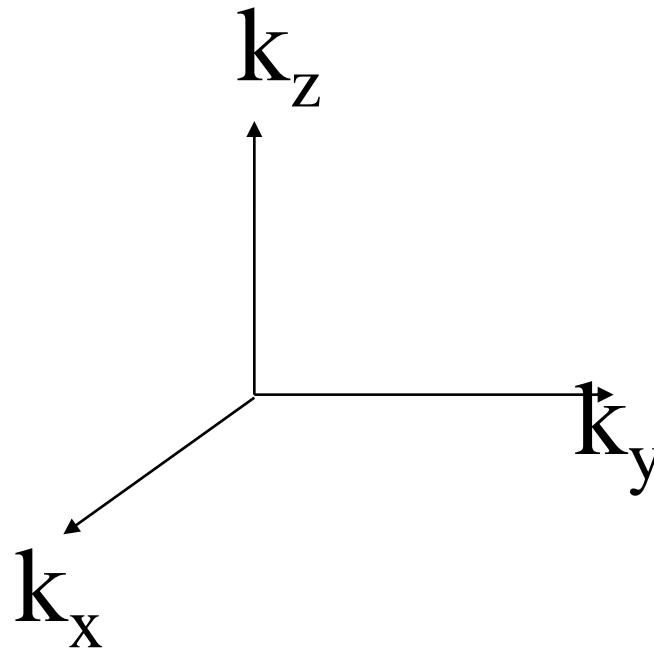
Number of states with energy between E and $E + dE$ *per volume*.

Density of states:

Easier first to think of in k-space:

Density of states in k-space is uniform:

One state per $(\pi/L)^3$:

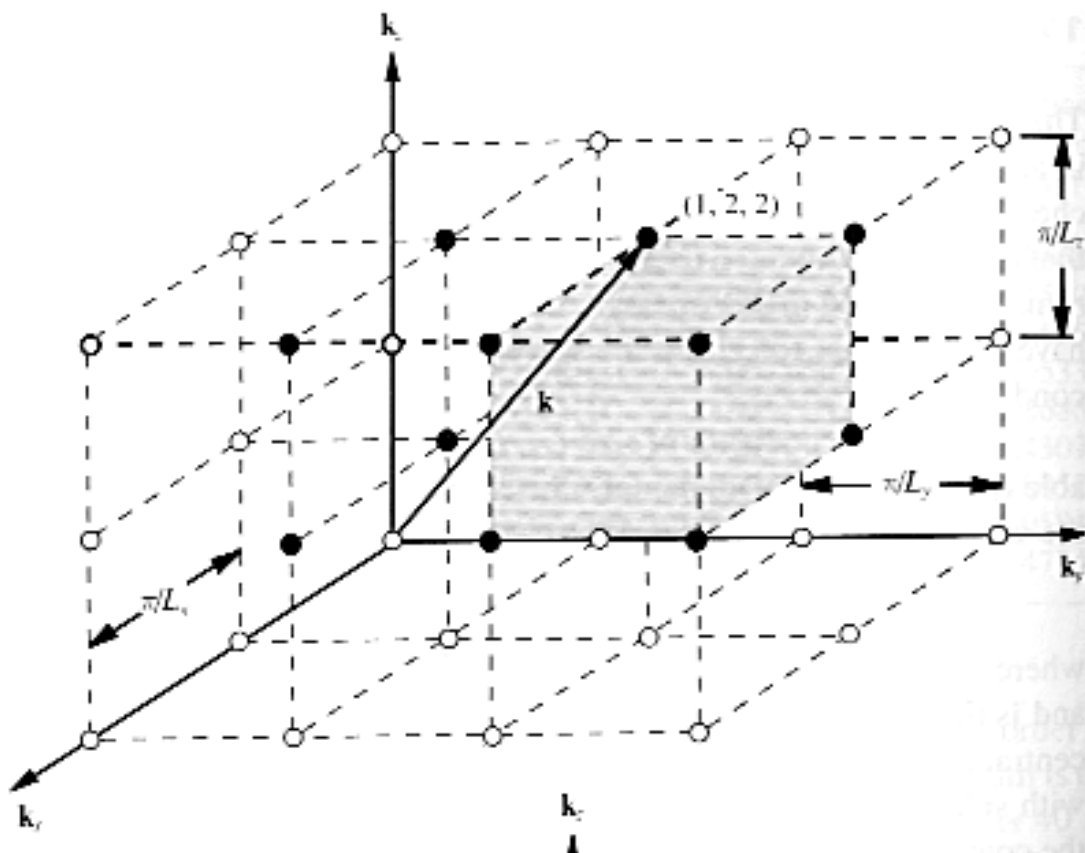


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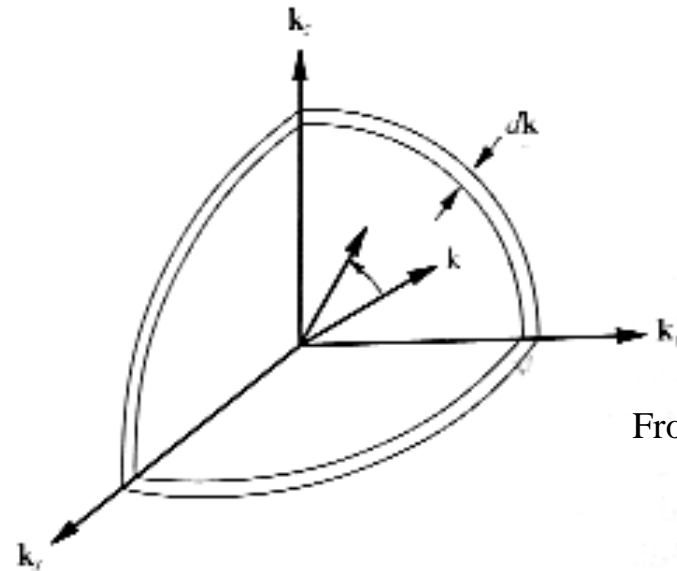
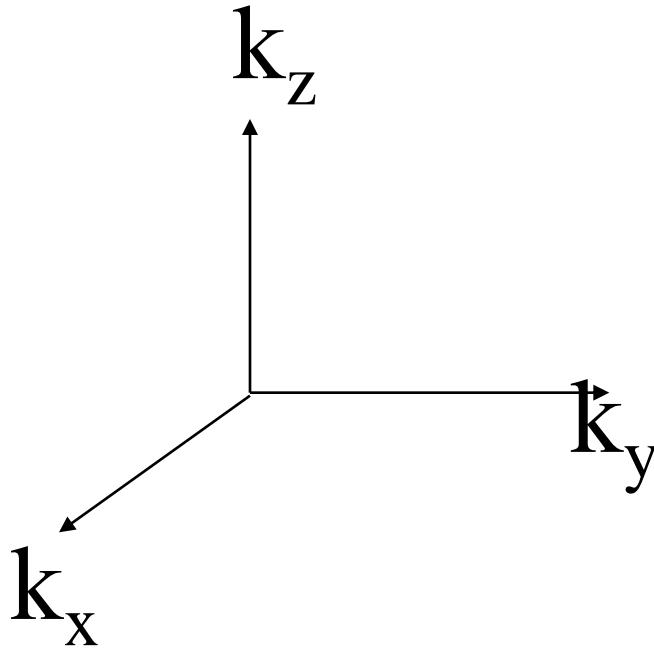


From Verdeyen

Density of states:

Number of states between k , $k+dk$:

$$N_k dk = ?$$



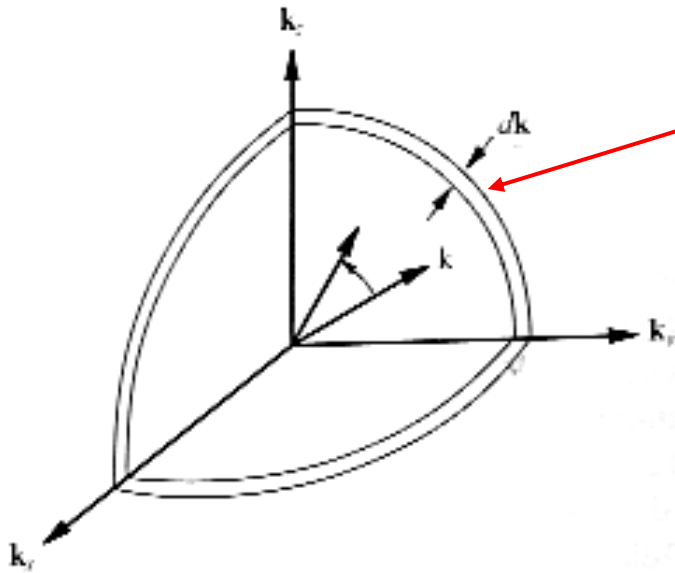
$$k \equiv \sqrt{k_x^2 + k_y^2 + k_z^2}$$

$$k_{n_x} = n_x \pi / L$$

$$k_{n_y} = n_y \pi / L$$

$$k_{n_z} = n_z \pi / L$$

$$N_k dk = ?$$



Volume of spherical shell
 $= 4\pi k^2 dk / 8$

8 is for upper right quadrant

Number of states in volume =
 Volume x States/volume

States/volume = $1 / (\pi/L)^3$:

$$N_k dk = \left(4\pi k^2 dk / 8 \right) \cdot \left(\frac{1}{(\pi/L)^3} \right) \cdot 2 = L^3 \frac{k^2 dk}{\pi^2}$$

$$\rho_k dk \equiv \frac{N_k dk}{\text{volume}} = \frac{k^2 dk}{\pi^2}$$

HW you will do calculation for 2 dimensional world.

$$\rho(E)dE = ?$$

We use:

$$\rho_k dk = \rho(E)dE$$

$$\rho_k dk = \frac{k^2 dk}{\pi^2}$$

$$E = \frac{\hbar^2 k^2}{2m} \Rightarrow k = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow dk = \sqrt{\frac{2m}{\hbar^2}} \frac{dE}{2\sqrt{E}}$$

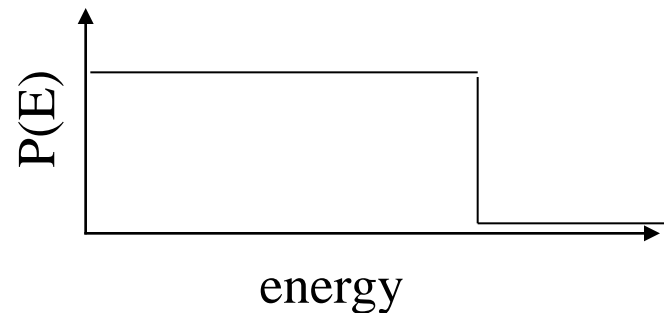
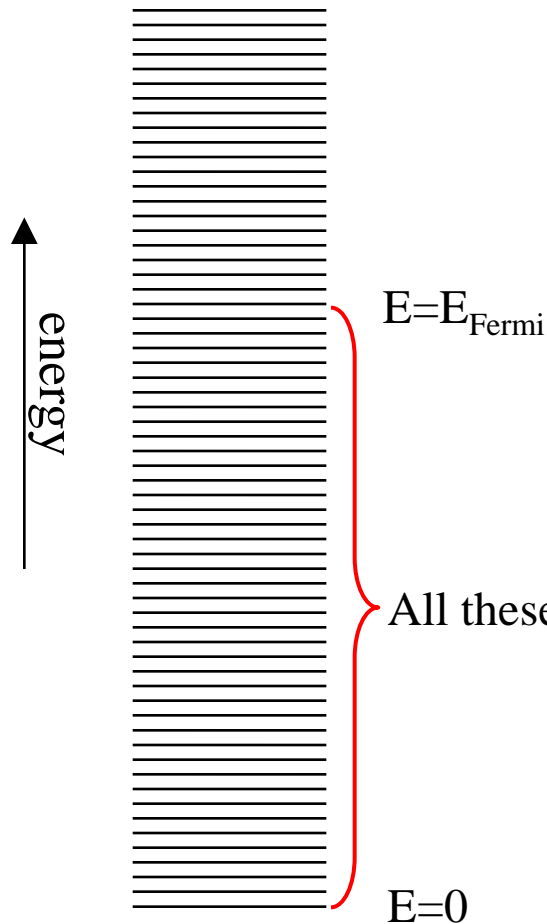
$$\rho(E)dE = \frac{2^{3/2} m^{3/2}}{2\pi^2 \hbar^3} \cdot E^{1/2} dE$$

Fermi gas:

At zero temperature, as we add electrons to the box, we gradually fill up all the states.
(DISCUSS PAULI EXCLUSION PRINCIPLE
-IMPORTANT!)

When we are done filling the box, the energy of the last electron is called the “Fermi energy.”

“Gas” means we neglect electron-electron interactions.

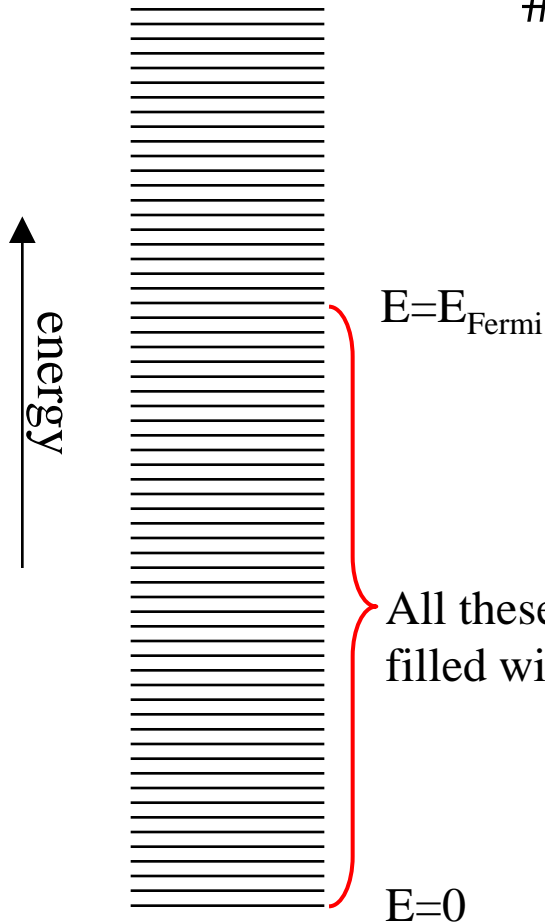


Fermi energy:

$$\# \text{ electrons} = \int_0^{E_f} N_E dE = \int_0^{E_f} L^3 \frac{2^{3/2} m^{3/2}}{2\pi^2 \hbar^3} \cdot E^{1/2} dE$$

$$\# \text{ electrons} = L^3 \frac{2^{3/2} m^{3/2}}{2\pi^2 \hbar^3} \cdot \frac{2}{3} E_f^{3/2}$$

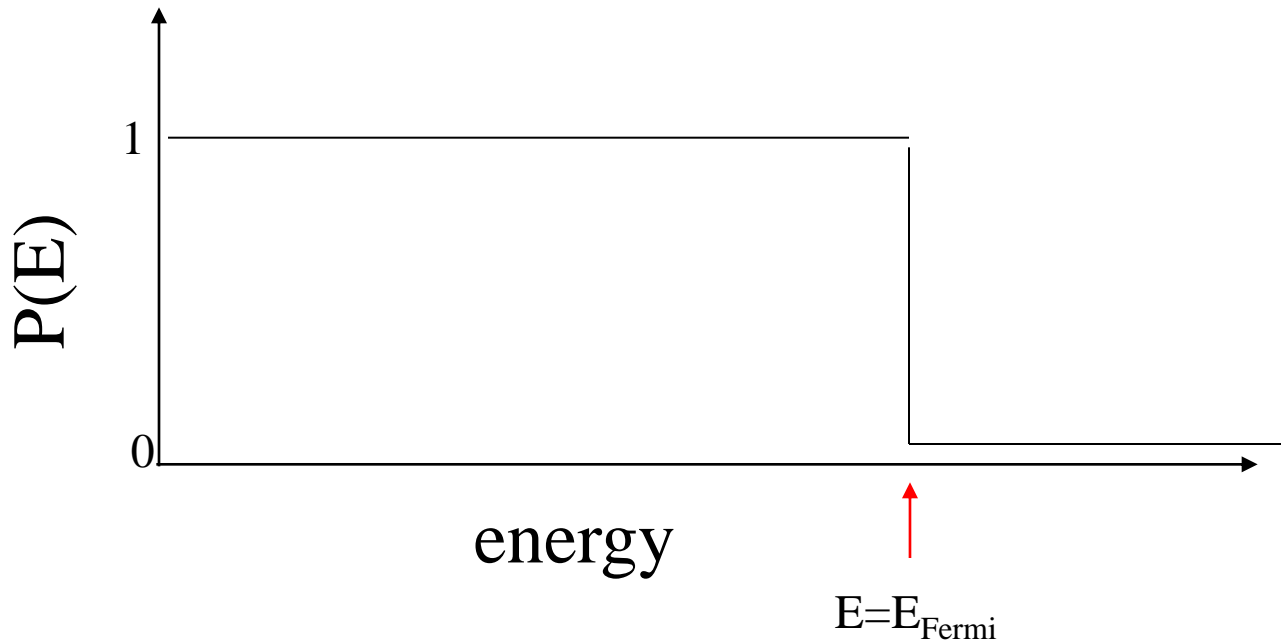
$$\Rightarrow E_f = \frac{\hbar^2 3^{2/3} \pi^{4/3}}{2m} \left(\frac{\# \text{ electrons}}{L^3} \right)^{2/3}$$



In a typical metal, $L \sim 0.1 \text{ nm}$.

$$E_f \sim 10 \text{ eV}$$

Occupation probability:



$P(E)$ = probability of occupying a state
with energy E

What about finite temperature?

Boltzmann:

Recall Boltzmann factor $P(\varepsilon)$:

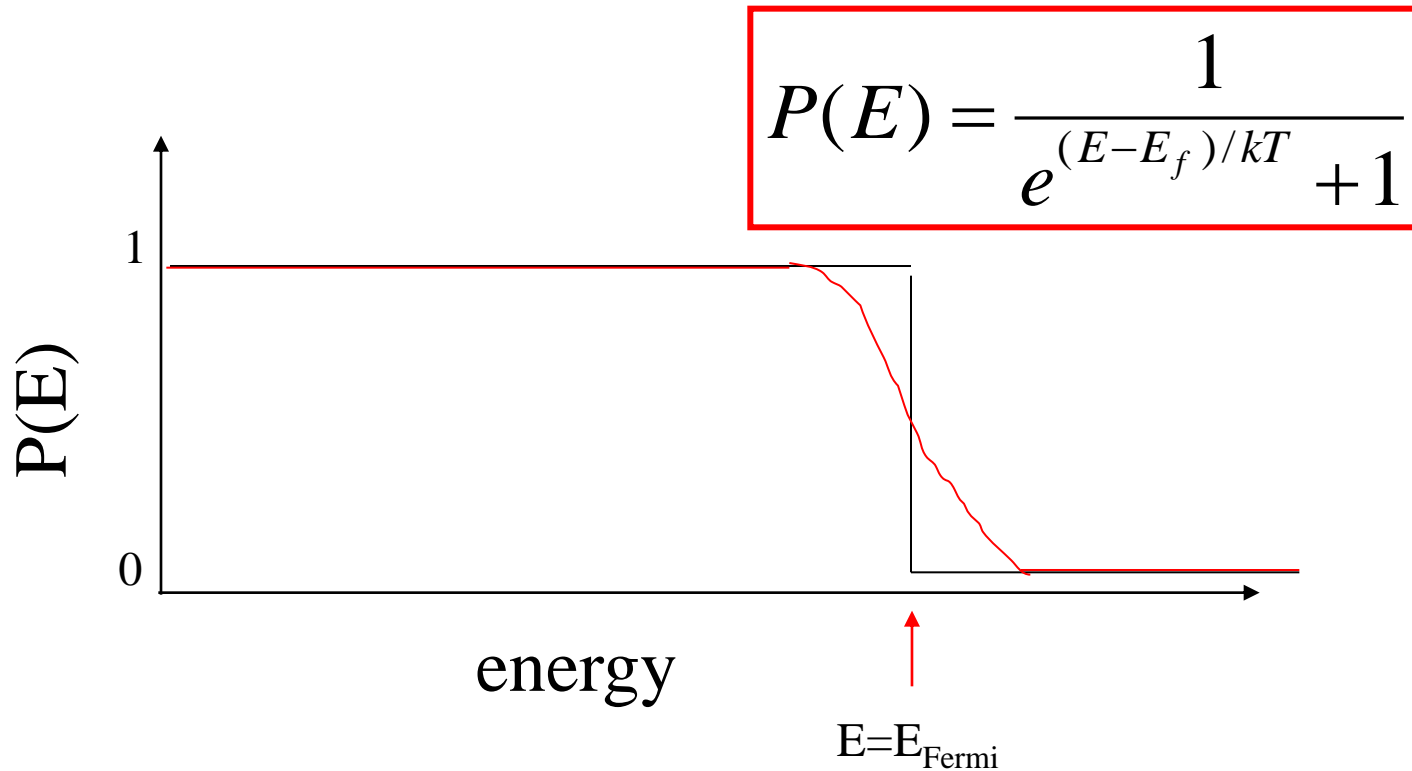
“The probability for a physical system to be in a state with energy ε is proportional to $e^{-\varepsilon/k_B T}$.”

This is actually not quite true. It is classical.
A quantum calculation shows for electrons:

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

Called Fermi-Dirac distribution function.
Boltzmann is high-energy limit (discuss!)

Fermi-Dirac:



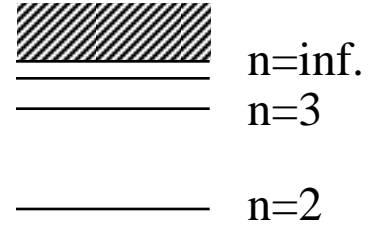
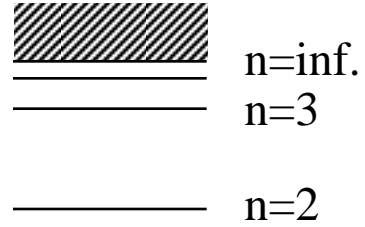
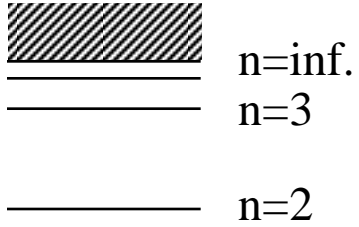
$P=1/2$ at E_f for all temperatures.

kT

Forget about free electrons for now.

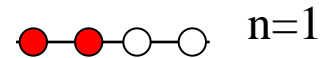
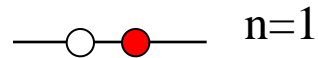
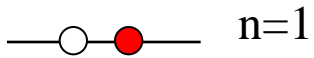
Back to the hydrogen atom.

Chemical bonds:

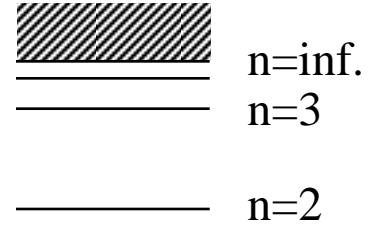
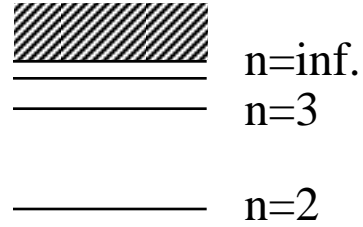
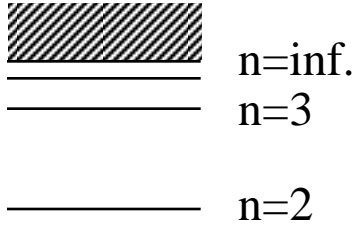


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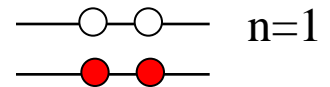
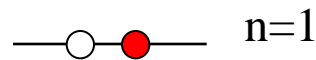
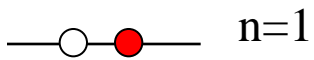


Chemical bonds:



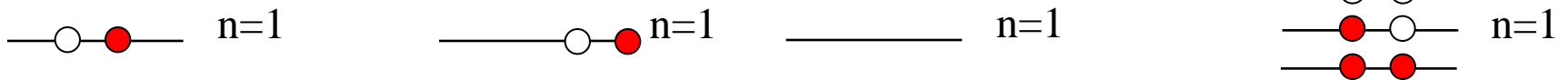
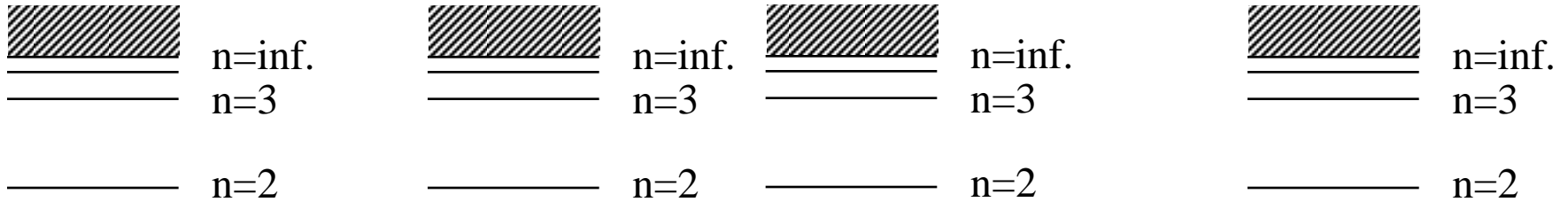
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“Bonding and anti-bonding”

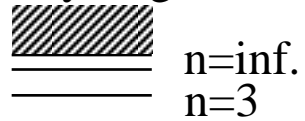
Chemical bonds:



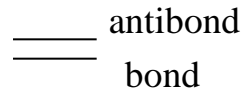
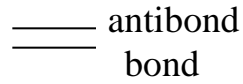
“N atoms give N levels”

Band theory of solids:

1 Hydrogen atom:



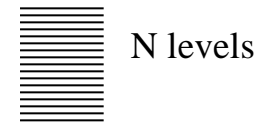
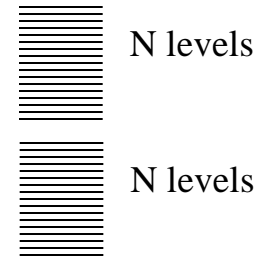
2 Hydrogen atoms:



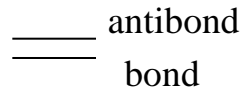
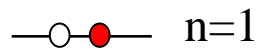
3 Hydrogen atoms:



N Hydrogen atoms:



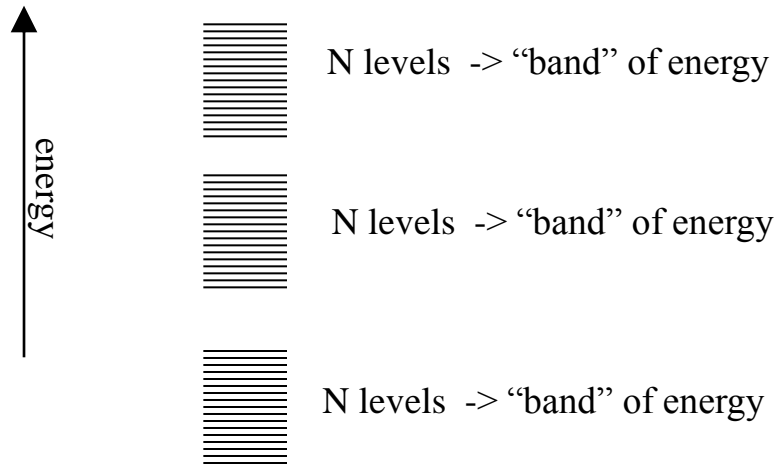
energy



Band theory of solids:

N Hydrogen atoms:

N \rightarrow infinity



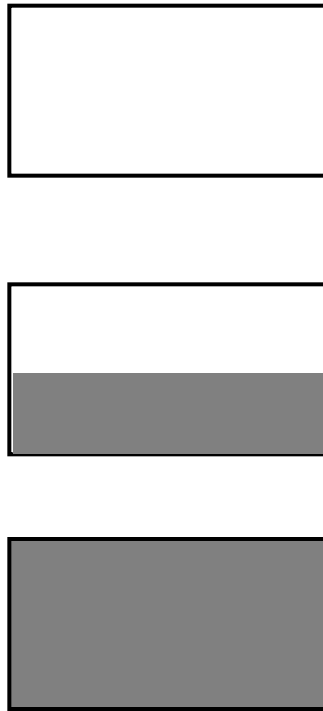
Band theory of solids:

Filled bands do not conduct electricity!

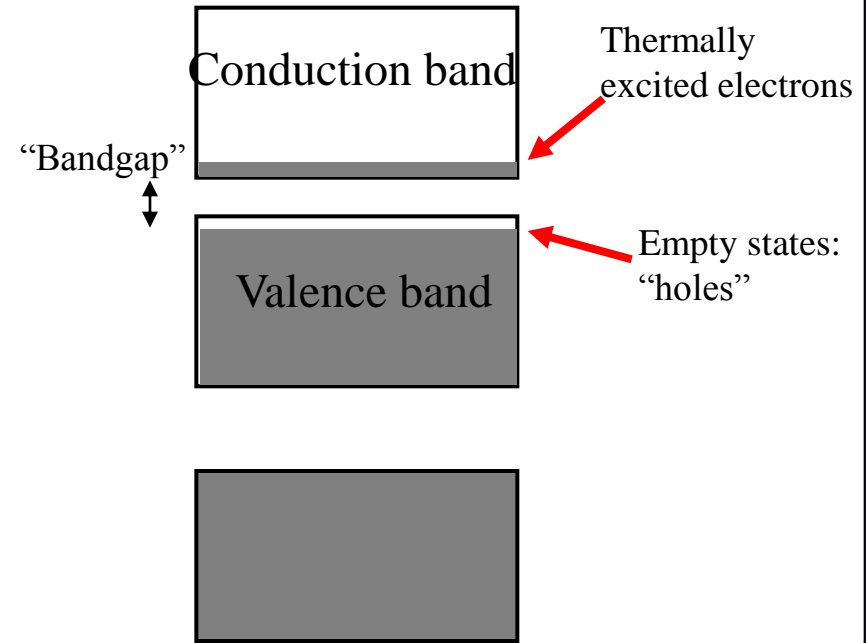
Insulator:



Metal:



Semiconductor:

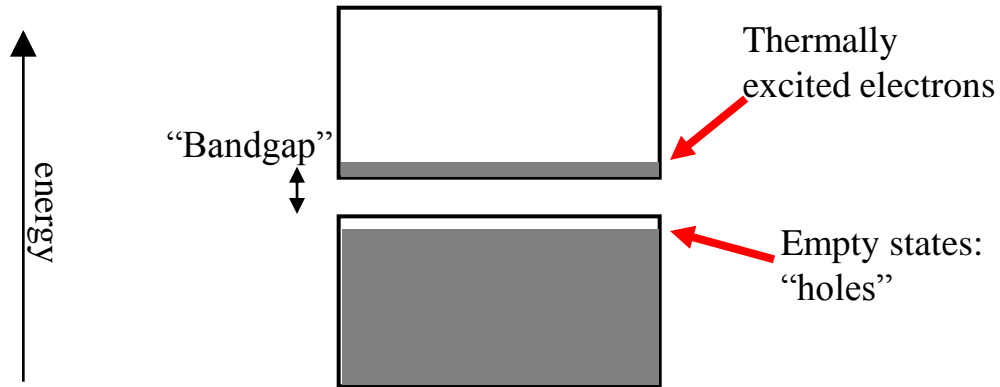


We usually don't care about lower bands.

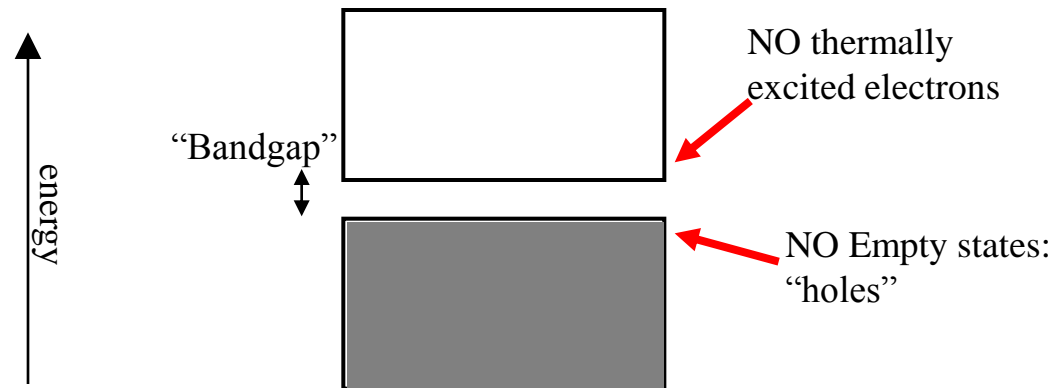
LASER will be formed by electrons going from conduction to valence band...

Semiconductors:

Finite temperature:



Zero temperature:



NO CONDUCTION
AT ZERO TEMPERATURE.
Only at finite temperature.
Hence the name, “semi”conductors.

Group**

Period

Silicon:

Gap = 1.1 eV

GaAs:

Gap = 1.4 eV

1	1 IA 1A 1 H 1.008	2 IIA 2A 4 Be 9.012											13 IIIA 3A 5 B 10.81	14 IVA 4A 6 C 12.01	15 VA 5A 7 N 14.01	16 VIA 6A 8 O 16.00	17 VIIA 7A 9 F 19.00	18 VIIIA 8A 10 Ne 20.18
2	3 Li 6.941	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
3	11 Na 22.99	20 Ca 40.08	3 IIIB 3B 21 Sc 44.96	4 IVB 4B 22 Ti 47.88	5 VB 5B 23 V 50.94	6 VIB 6B 24 Cr 52.00	7 VIIB 7B 25 Mn 54.94	8 VIII 8 26 Fe 55.85	9 VIII 8 27 Co 58.47	10 VIII 8 28 Ni 58.69	11 IB 11 29 Cu 63.55	12 IIB 12 30 Zn 65.39	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
4	19 K 39.10	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
5	37 Rb 85.47	88 Ba 137.3	57 La* 138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.9	75 Re 186.2	76 Os 190.2	77 Ir 190.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.5	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
6	55 Cs 132.9	88 Ba 137.3	57 La* 138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.9	75 Re 186.2	76 Os 190.2	77 Ir 190.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.5	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (210)	85 At (210)	86 Rn (222)
7	87 Fr (223)	88 Ra (226)	89 Ac~ (227)	104 Rf (257)	105 Db (260)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 --- ()	111 --- ()	112 --- ()	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (210)	85 At (210)	86 Rn (222)

Lanthanide Series*

58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (147)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
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From <http://pearl1.lanl.gov/periodic/default.htm>

Actinide Series~

90 Th 232.0	91 Pa (231)	92 U (238)	93 Np (237)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (249)	99 Es (254)	100 Fm (253)	101 Md (256)	102 No (254)	103 Lr (257)
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Remember free electrons now.

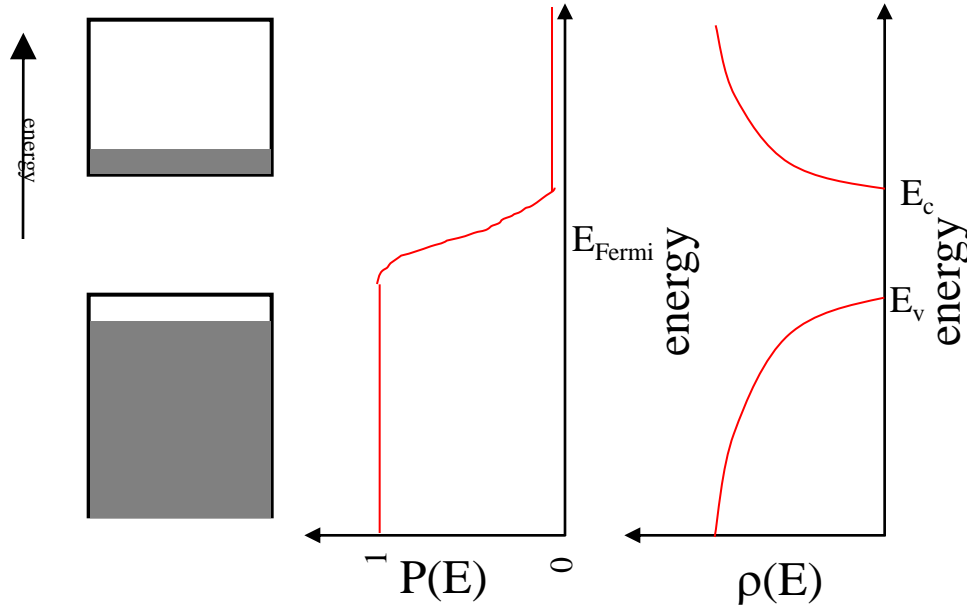
Even though electrons in a semiconductor live in “bands of energy”, we can treat them like free electrons, except for the gap.

The price we pay for treating a complicated system like free electrons:

- 1) E_{Fermi} is in the middle of the gap.
- 3) Density of states origin is referred to edge of band.
- 2) Electrons, holes have different “effective” mass values.

We now discuss these three points:

How many electrons in conduction band?



$$n_i = \int_{E_c}^{\infty} P(E) \rho(E) dE$$

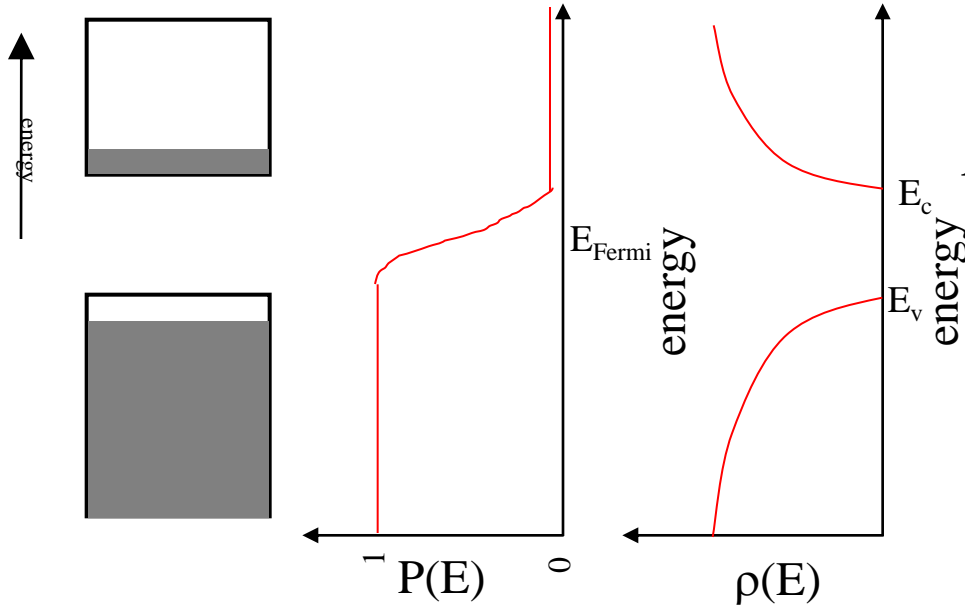
$$\rho_{electrons}(E) dE = \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^3} \cdot (E - E_c)^{1/2} dE$$

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

(Discuss high energy appr. on board.)

$$n_i = 2 \left(\frac{m_e^* kT}{2\pi \hbar^2} \right)^{3/2} e^{(E_f - E_c)/kT}$$

How many holes in valence band?



$$p_i = \int_{E_c}^{-\infty} [1 - P(E)] \rho(E) dE$$

$$\rho_{electrons}(E) dE = \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^3} \cdot (E - E_c)^{1/2} dE$$

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

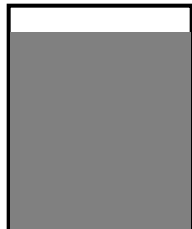
$$p_i = 2 \left(\frac{m_h^* kT}{2\pi \hbar^2} \right)^{3/2} e^{(E_v - E_f)/kT}$$

Holes and electrons

↑ energy



$$p_i = 2 \left(\frac{m_h^* kT}{2\pi\hbar^2} \right)^{3/2} e^{(E_v - E_f)/kT} \equiv N_v e^{(E_v - E_f)/kT}$$



$$n_i = 2 \left(\frac{m_e^* kT}{2\pi\hbar^2} \right)^{3/2} e^{(E_f - E_c)/kT} \equiv N_c e^{(E_f - E_c)/kT}$$

But $E_f - E_c = (1/2) E_{\text{gap}}$ and $E_v - E_f = (1/2) E_{\text{gap}}$.

With some algebra,

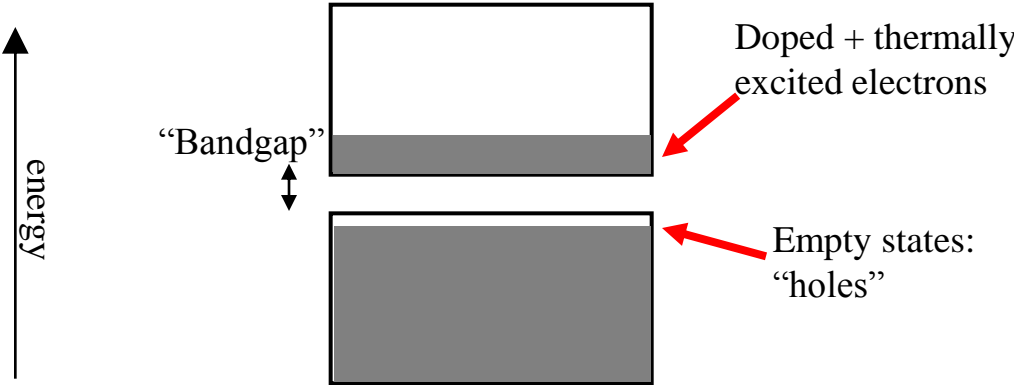
$$n_i = p_i = 2 \left(\frac{kT}{2\pi\hbar^2} \right)^{3/2} (m_e^* m_h^*)^{3/4} e^{-E_g/2kT}$$

$$n_i \sim 10^6 \text{ cm}^{-3} (\text{GaAs})$$

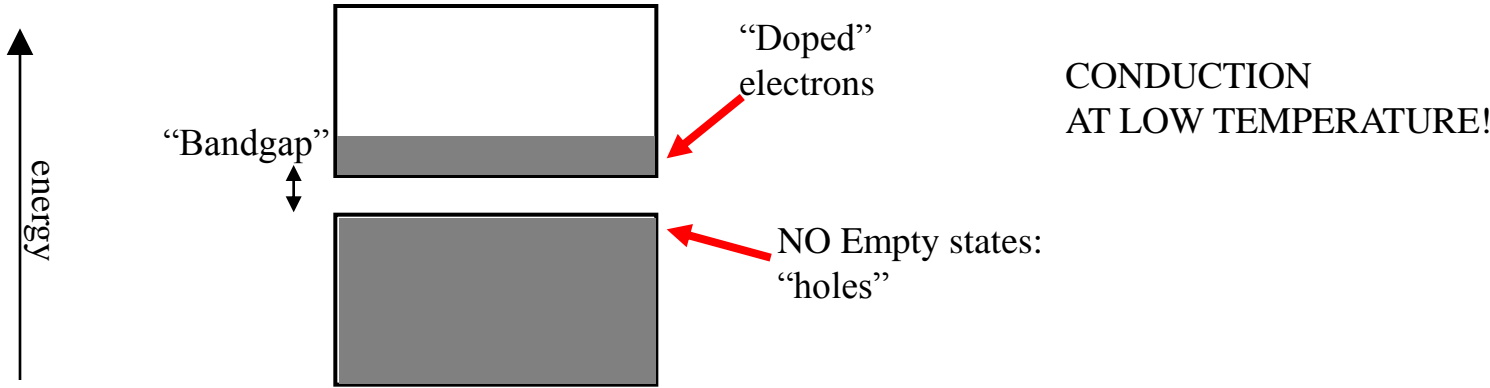
$$n_i \sim 10^{10} \text{ cm}^{-3} (\text{Si})$$

n-type doped semiconductors:

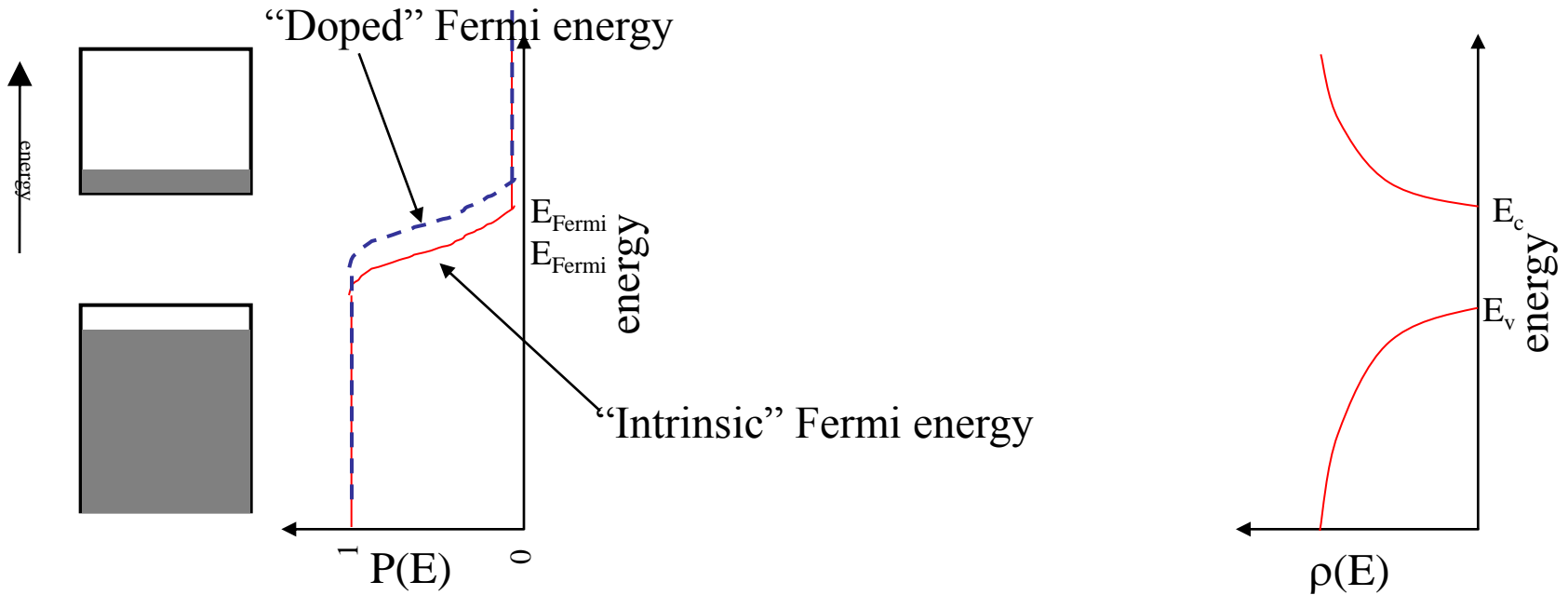
Finite temperature:



“Low” temperature:



How many electrons in conduction band?



“Law of mass action”

$$n \cdot p = n_i^2 = N_c N_v e^{-E_g/kT}$$

$$p - n = N_{acceptors} - N_{donors}$$

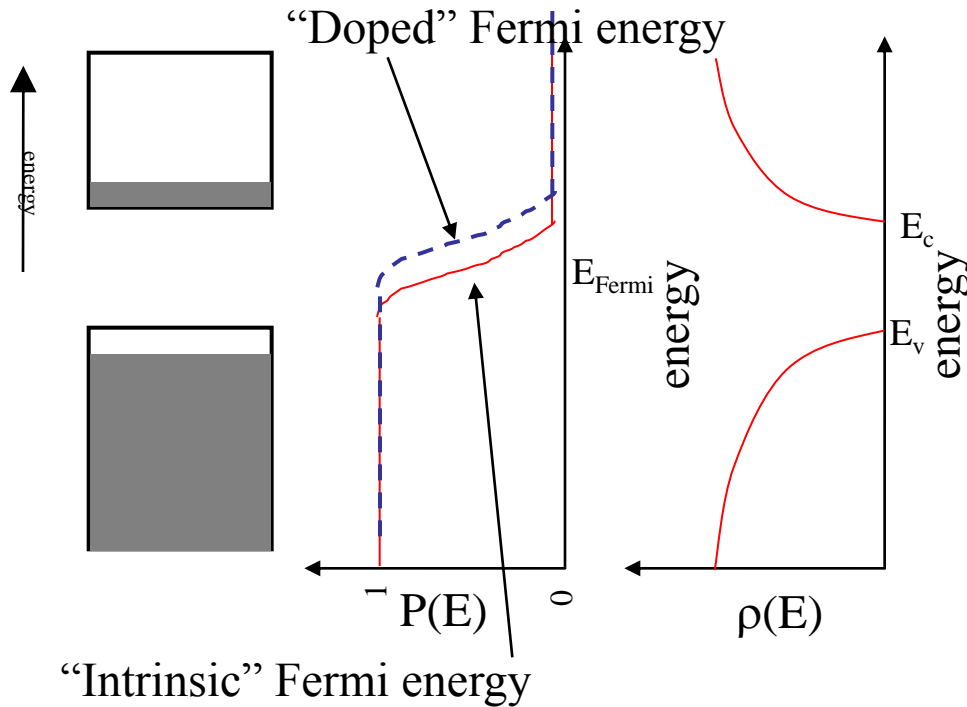
$$p - n = N_d$$

$$n_i^2 / n - n = N_d$$

$$n = \frac{\sqrt{N_d^2 + 4n_i^2} + N_d}{2} \approx N_d$$

How many electrons in conduction band?

A method to calculate if E_{fermi} is known:



$$n = \int_{E_c}^{\infty} P(E) \rho(E) dE$$

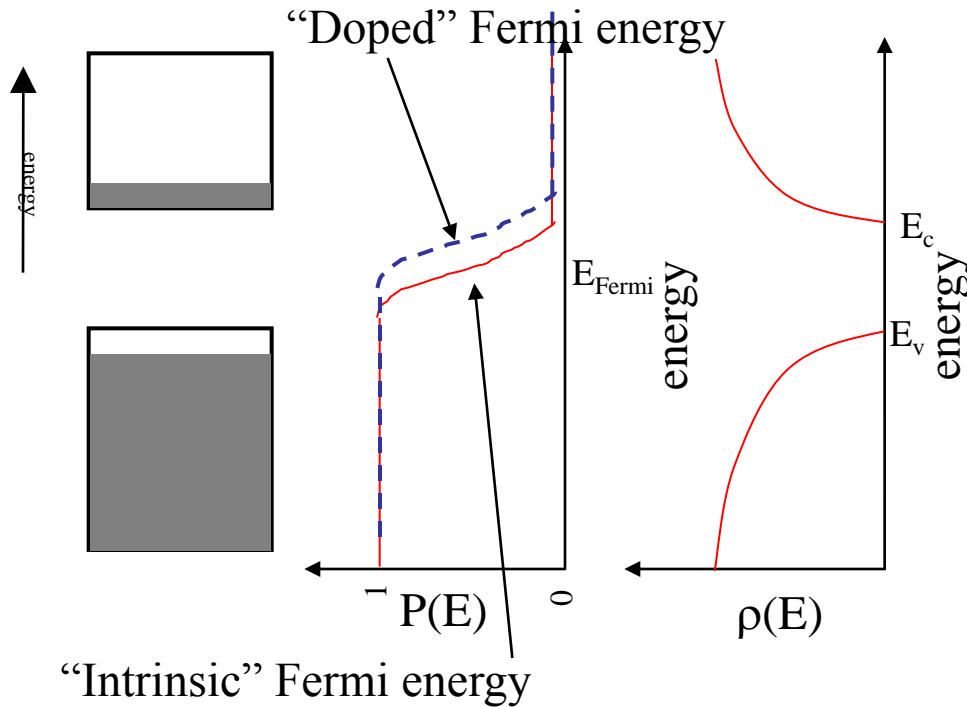
$$\rho_{\text{electrons}}(E) dE = \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^3} \cdot (E - E_c)^{1/2} dE$$

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

$$n = 2 \left(\frac{m_e^* kT}{2\pi \hbar^2} \right)^{3/2} e^{(E_f - E_c)/kT}$$

How many holes in valence band?

A method to calculate if E_{fermi} is known:



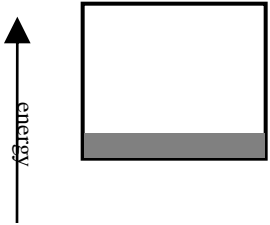
$$p = \int_{E_c}^{-\infty} [1 - P(E)] \rho(E) dE$$

$$\rho_{\text{electrons}}(E) dE = \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^3} \cdot (E - E_c)^{1/2} dE$$

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

$$p = 2 \left(\frac{m_h^* kT}{2\pi\hbar^2} \right)^{3/2} e^{(E_v - E_f)/kT}$$

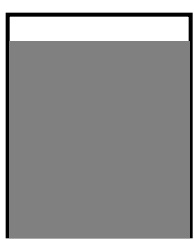
Holes and electrons when doped n-type



energy ↑

A diagram showing a rectangular energy band with a small shaded region at the bottom, representing the valence band in a doped n-type semiconductor. An upward-pointing arrow labeled 'energy' is to the left.

$$p = 2 \left(\frac{m_h^* kT}{2\pi\hbar^2} \right)^{3/2} e^{(E_v - E_f)/kT}$$



A diagram showing a rectangular energy band with a large shaded region at the bottom and a small unshaded region at the top, representing the conduction band in a doped n-type semiconductor.

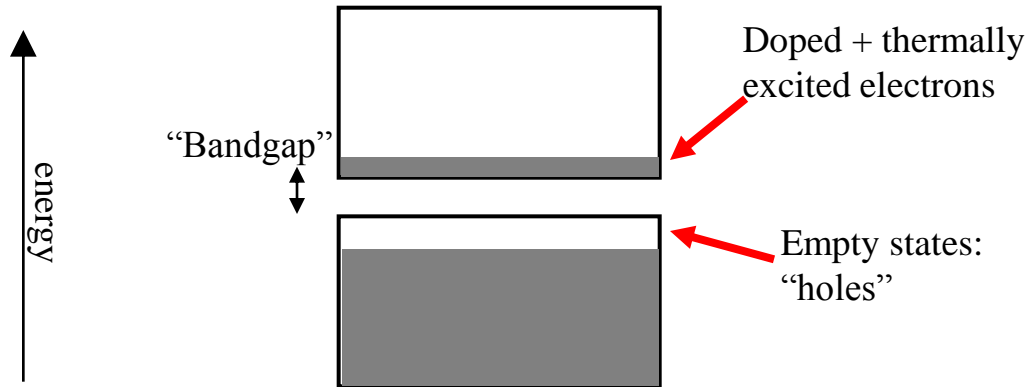
$$n = 2 \left(\frac{m_e^* kT}{2\pi\hbar^2} \right)^{3/2} e^{(E_f - E_c)/kT}$$

But $E_f - E_c \neq (1/2) E_{\text{gap}}$ and $E_v - E_f \neq (1/2) E_{\text{gap}}$!

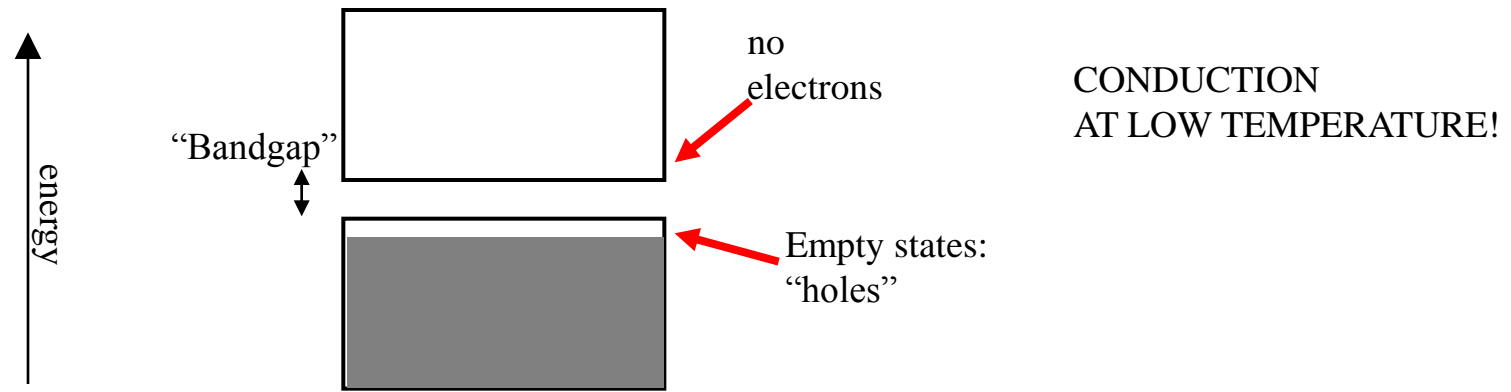
$$n > p$$

p-type doped semiconductors:

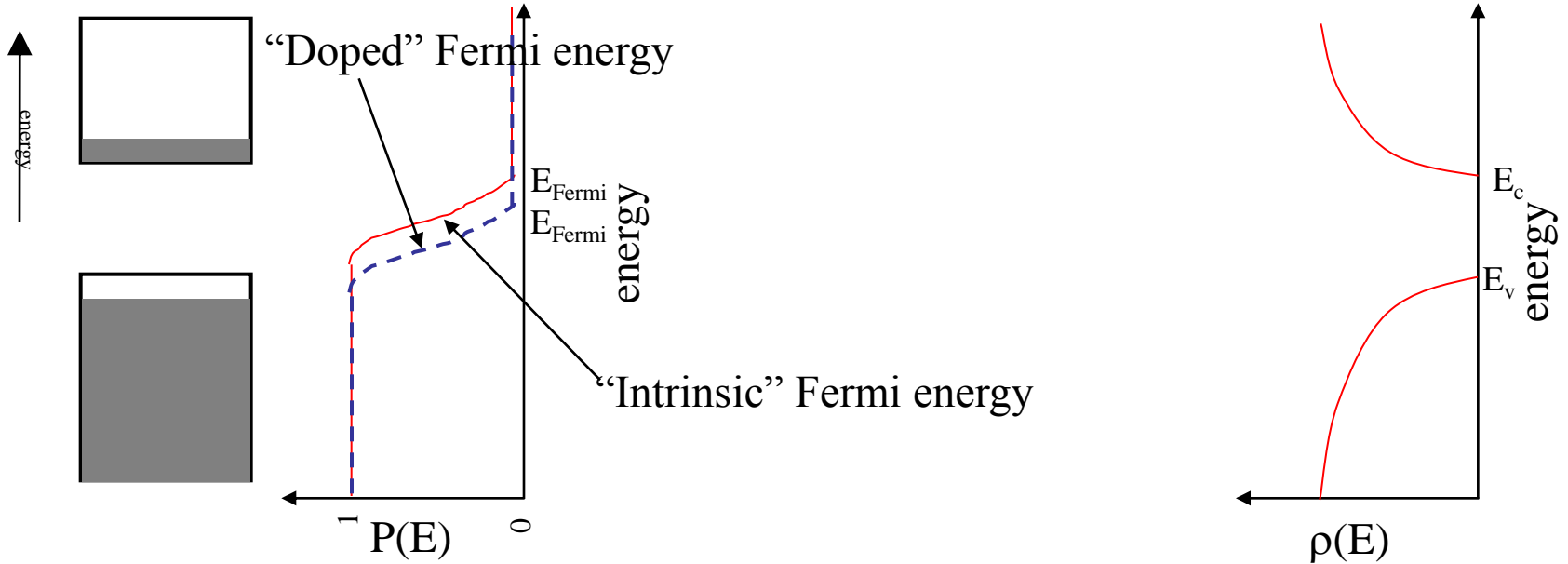
Finite temperature:



"Low" temperature:



How many holes in valence band?



$$n \cdot p = n_i^2$$

$$p - n = N_{acceptors} - N_{donors}$$

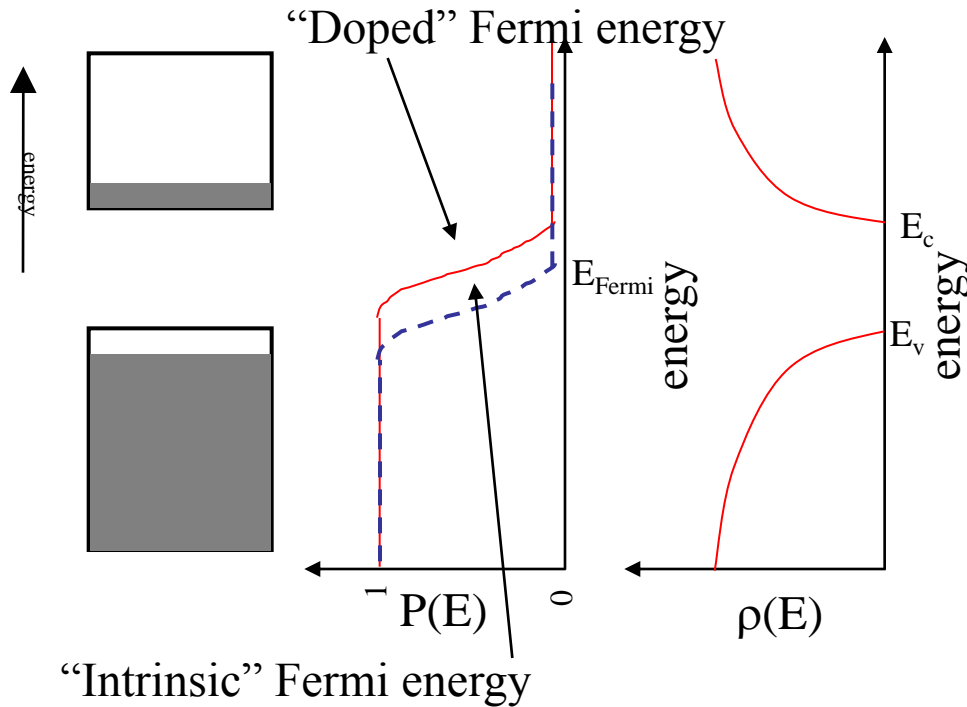
$$p - n = N_a$$

$$p - n_i^2 / p = N_a$$

$$p = \frac{\sqrt{N_a^2 + 4n_i^2} + N_a}{2} \approx N_a$$

How many holes in valence band?

A method to calculate if E_{fermi} is known:



$$p = \int_{E_c}^{-\infty} [1 - P(E)] \rho(E) dE$$

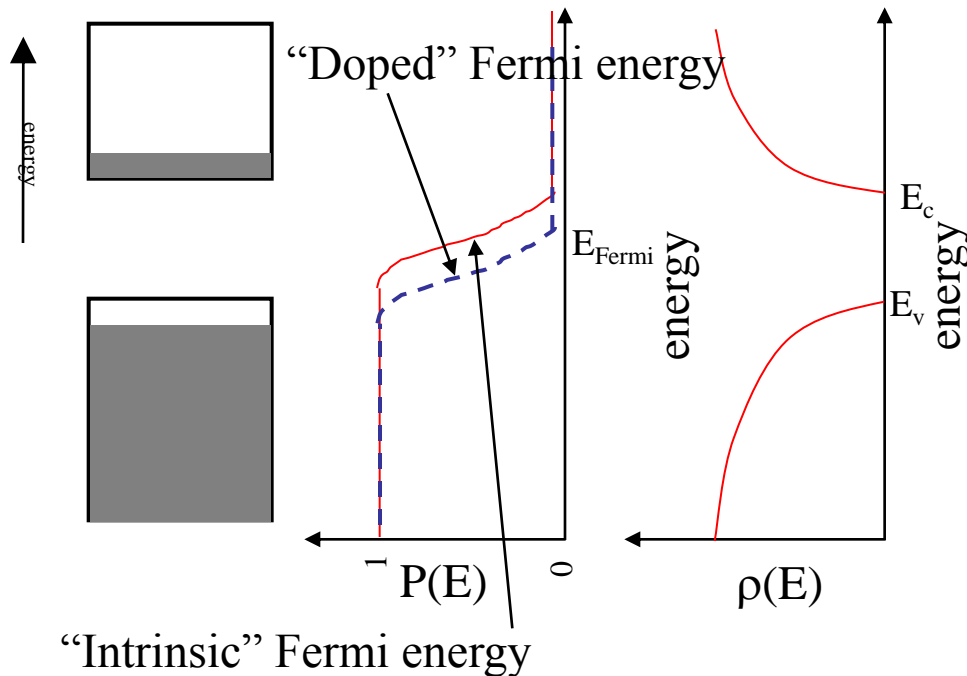
$$\rho_{\text{electrons}}(E) dE = \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^3} \cdot (E - E_c)^{1/2} dE$$

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

$$p = 2 \left(\frac{m_h^* kT}{2\pi\hbar^2} \right)^{3/2} e^{(E_v - E_f)/kT}$$

How many electrons in conduction band?

A method to calculate if E_{fermi} is known:



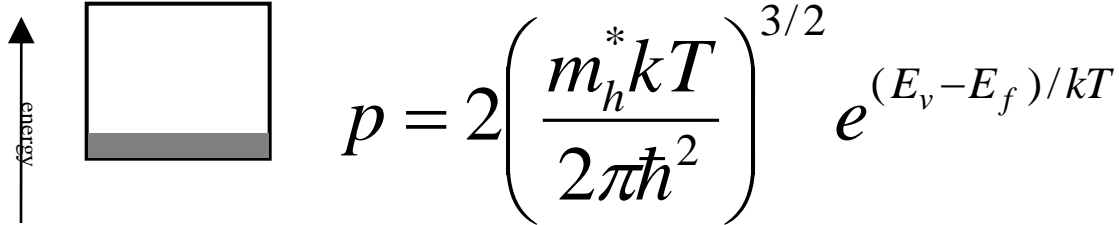
$$n = \int_{E_c}^{\infty} P(E) \rho(E) dE$$

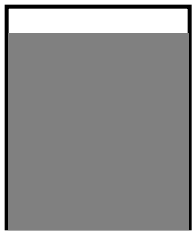
$$\rho_{\text{electrons}}(E) dE = \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^3} \cdot (E - E_c)^{1/2} dE$$

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

$$n = 2 \left(\frac{m_e^* kT}{2\pi\hbar^2} \right)^{3/2} e^{(E_f - E_c)/kT}$$

Holes and electrons when doped


$$p = 2 \left(\frac{m_h^* k T}{2 \pi \hbar^2} \right)^{3/2} e^{(E_v - E_f) / k T}$$

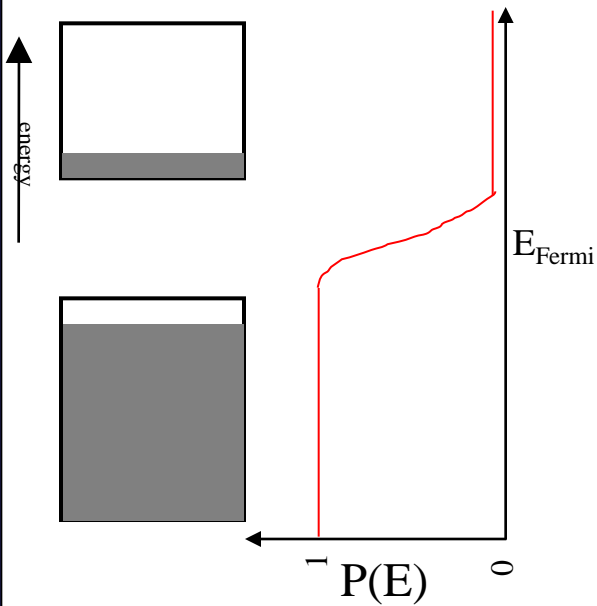

$$n = 2 \left(\frac{m_e^* k T}{2 \pi \hbar^2} \right)^{3/2} e^{(E_f - E_c) / k T}$$

But $E_f - E_c \neq (1/2) E_{\text{gap}}$ and $E_v - E_f \neq (1/2) E_{\text{gap}}$!

$$n < p$$

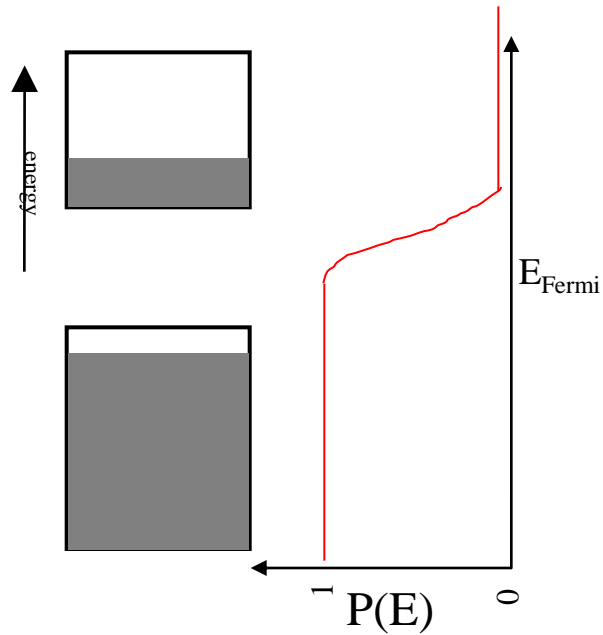
In conclusion:

Intrinsic:



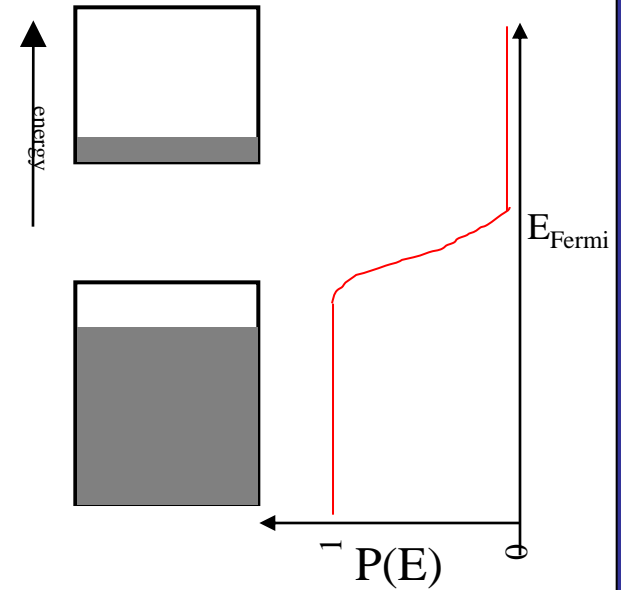
$$n = p$$

n-type:



$$n > p$$

p-type:



$$n < p$$

What we've done:

- Free electron density of states
- Fermi-Dirac distribution function
- Band theory of solids (metal, insulator, semiconductor)
- Effective mass, density of states in semiconductors
- Electron, hole carrier concentrations in semiconductors