Lecture 12: Free electrons

- Quantum mechanics
- Free electrons in a box
- Fermi gas
- Fermi-Dirac distribution function
- Covers Verdeyen ch. 11
- Please ask questions!

Free electron theory of solids

- Each atom in the solid "gives up" one electron
- Each electron is free to move where-ever it wants, with no scattering
- Completely the opposite of atom lasers, where each electron is bound to each atom
- Amazingly, this simple idea makes predictions that are true!
- Not for semiconductors, but metals
- Still need to understand this for semiconductors

Electrons are waves, too.

Quantum mechanics of free particles:

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

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:

$\omega = E/\hbar$

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

Momentum:

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

Energy:

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

Schrodinger equation:

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

(1 dimension)

(Time dependent)

Let $\Psi(x,t) = A\cdot e^{i(kx-\omega t)}$ A is a (complex) constant.

Then

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}A\cdot e^{i(kx-\omega t)} = i\hbar(-i\omega)A\cdot e^{i(kx-\omega t)}$$

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

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

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

Schrodinger equation:

(3 dimensions)

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

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

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:

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

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

$$= \frac{\hbar^2k^2}{2m}\left(A\cdot e^{i(\vec{k}\cdot\vec{r}-\omega t)}\right) = \frac{p^2}{2m}\Psi(\vec{r},t)$$

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

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

$$= A\cdot e^{i\left((k_x\cdot x+k_y\cdot y+k_z\cdot z)-\omega t\right)} = \underbrace{A\cdot e^{i(k_x\cdot x+k_y\cdot y+k_z\cdot z)}}_{\text{Call this } \psi(\vec{r})}\cdot e^{-i\omega t}$$

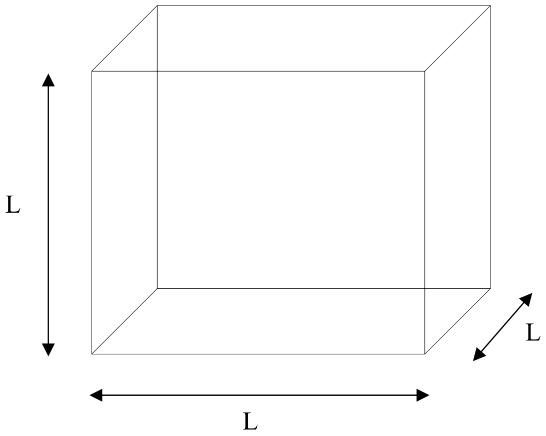
$$\Rightarrow \Psi(\vec{r},t) = \psi(\vec{r})\cdot e^{-i\omega t}$$

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

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

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

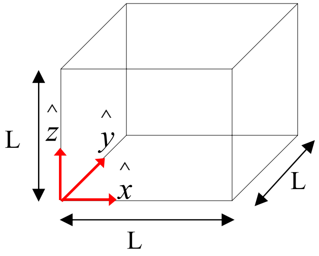
Confined particles: A box



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

Similar to electric field inside the box.

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



Everywhere outside the box

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

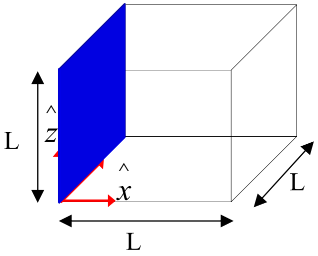
In particular,

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

on the boundaries.

As before, we will consider all six surfaces:

Boundary conditions:



The plane x=0:

Try:

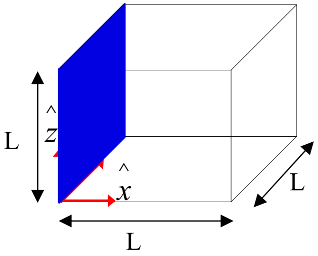
$$\psi(\vec{r}) = A\cdot e^{i(k_x\cdot x + k_y\cdot y + k_z\cdot z)}$$

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

Does not solve boundary condition!!!

Boundary conditions:

The plane x=0:



Let's try something:

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

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

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

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

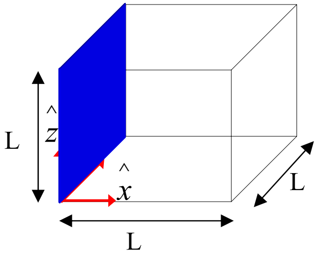
$$\psi(x=0,y,z) = A\cdot\left(e^{ik_x\cdot \underset{0}{\cancel{x}}} - e^{-ik_x\cdot \underset{0}{\cancel{x}}}\right)\cdot e^{i(k_y\cdot y + k_z\cdot z)}$$

$$= A\cdot\left(e^0 - e^0\right)\cdot e^{i(k_y\cdot y + k_z\cdot z)} = 0$$

Does solve boundary condition!!!

Boundary conditions:

The plane x=L:



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

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

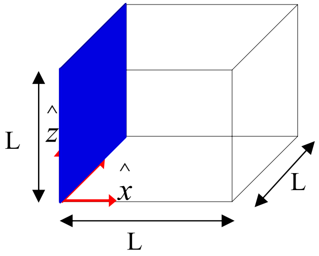
$$\boxed{\sin(\theta) = \frac{1}{2i}\left(e^{i\theta} - e^{-i\theta}\right)}$$

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

If and only if:

$$\boxed{k_n = n\pi / L}$$

Boundary conditions:



We can do the same for y, z:

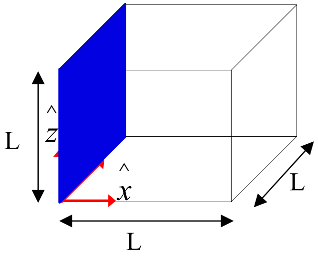
$$\psi(\vec{r}) = (2i)^3 A\cdot\sin(k_{n_x} x)\cdot\sin(k_{n_y} y)\cdot\sin(k_{n_z} z)$$

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

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

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

Many electrons:

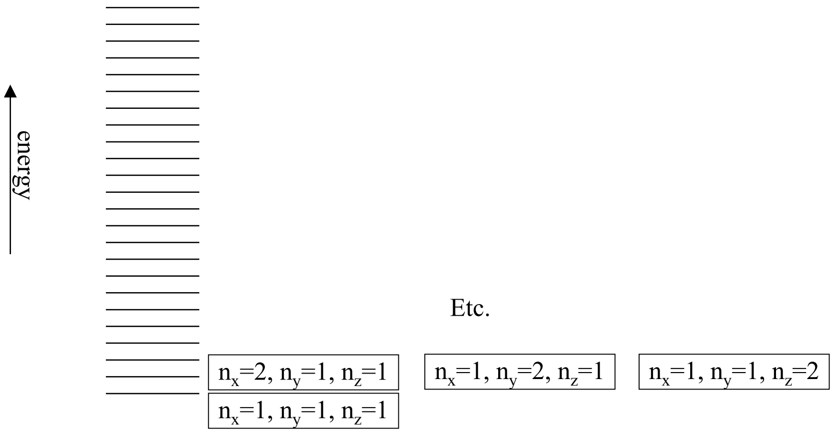


$$E = \frac{\hbar^2(\pi / L)^2}{2m}({n_x}^2 + {n_y}^2 + {n_z}^2)$$

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:



Etc.

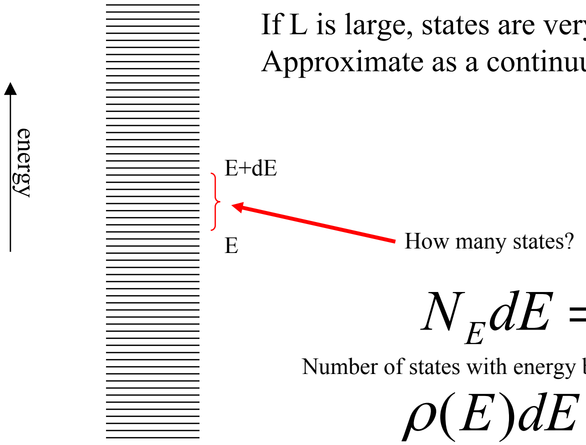
n_x=2, n_y=1, n_z=1

n_x=1, n_y=2, n_z=1

n_x=1, n_y=1, n_z=2

n_x=1, n_y=1, n_z=1

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

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

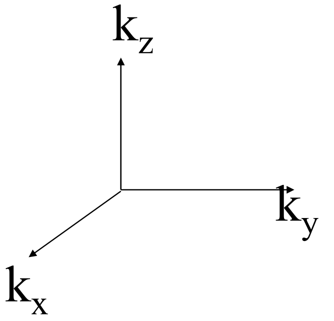
Number of states with energy between E and E + dE *per volume.*

Density of states:

Easier first to think of in k-space:

Density of states in k-space is uniform:

One state per (π/L)^3:



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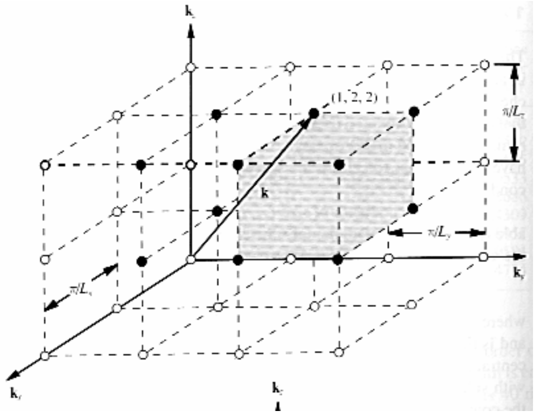
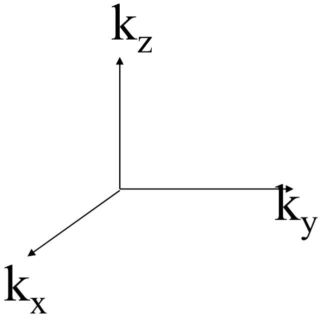


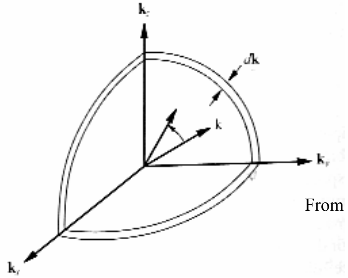
From Verdeyen

Density of states:

Number of states between k, k+dk:

$$N_k dk = ?$$





From Verdeyen

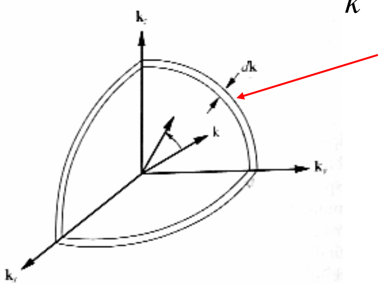
$$k_{n_x} = n_x \pi / L$$

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

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

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

$N_k dk = ?$



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 / $(\pi/L)^3$:

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

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

HW you will do calculation for 2 dimensional world.

$\rho(E)dE = ?$

We use:

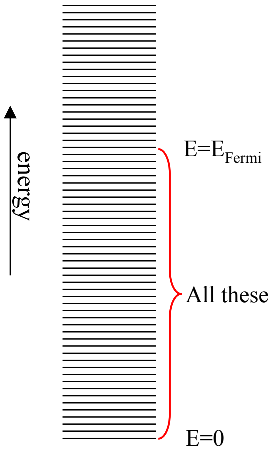
$$\rho_k dk = \rho(E)dE$$

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

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

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

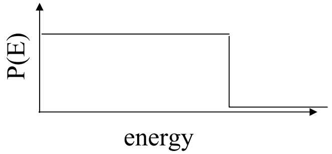
Fermi gas:



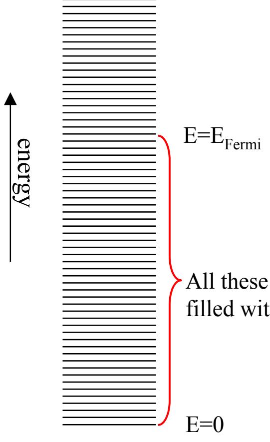
At zero temperature, as we add electrons to the box, we gradually fill up all the states. (DISCUSS PAULI EXCLUSION PRINCIPLE -IMPORTANT!)

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:



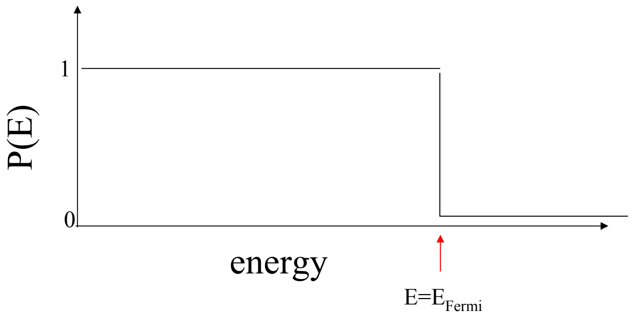
$$\#\,\text{electrons} = \int_0^{E_f} N_{\mathrm{E}}\mathrm{d}\mathrm{E} = \int_0^{E_f} L^3\,\frac{2^{1/2}m^{3/2}}{\pi^2\hbar^{3/2}}\cdot E^{1/2}dE$$

$$\#\,\text{electrons} = L^3\,\frac{2^{1/2}m^{3/2}}{\pi^2\hbar^{3/2}}\,\frac{2}{3}\,E_f^{3/2}$$

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

In a typical metal, L ~ 0.1 nm.
E_f ~ 10 eV

Occupation probability:



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

What about finite temperature?

Boltzmann:

Recall Boltzmann factor P(ε):

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

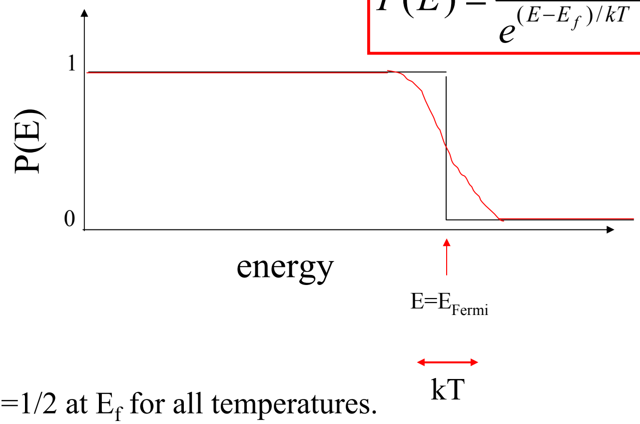
This is actually not quite true. It is classical. A quantum calculation shows for electrons:

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

Called Fermi-Dirac distribution function.

Fermi-Dirac:

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

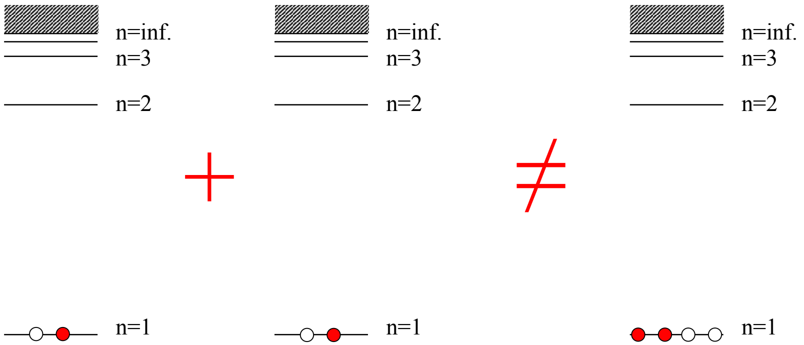


P=1/2 at E_f for all temperatures.

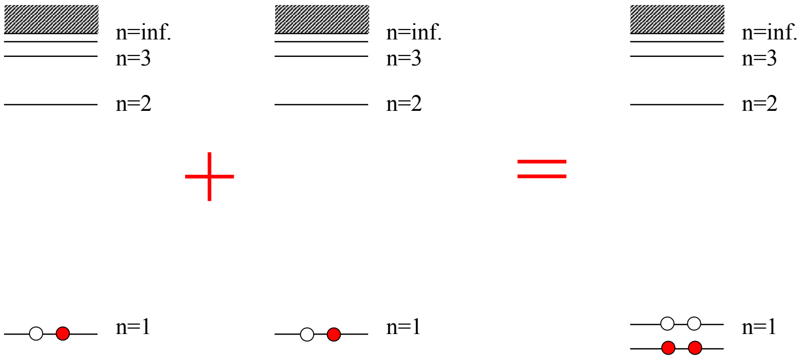
Forget about free electrons for now.

Back to the hydrogen atom.

Chemical bonds:

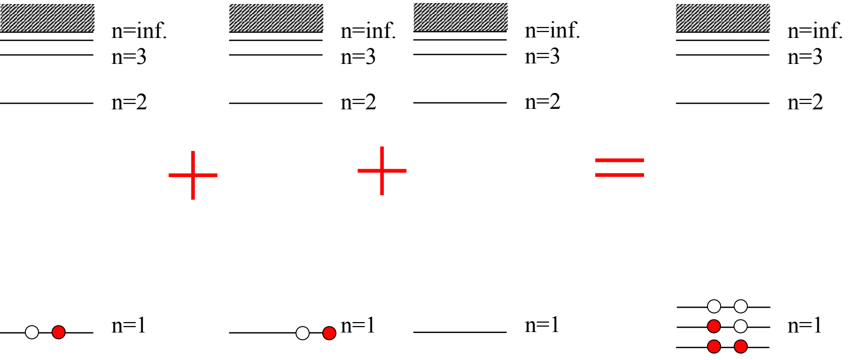


Chemical bonds:



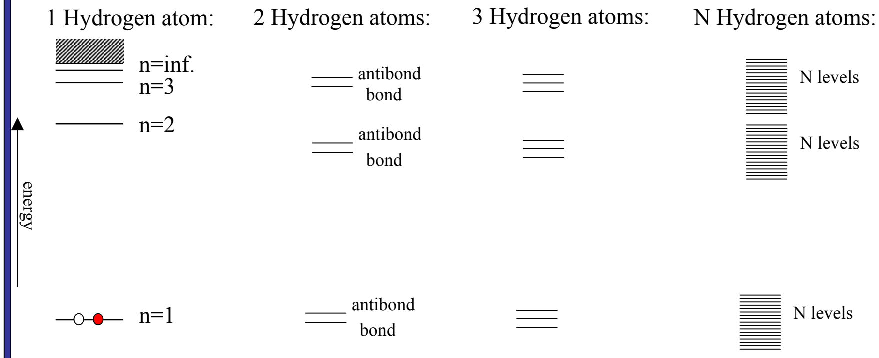
“Bonding and anti-bonding”

Chemical bonds:



“N atoms give N levels”

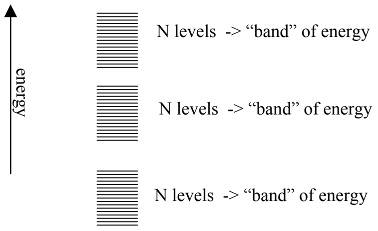
Band theory of solids:



Band theory of solids:

N Hydrogen atoms:

N -> infinity



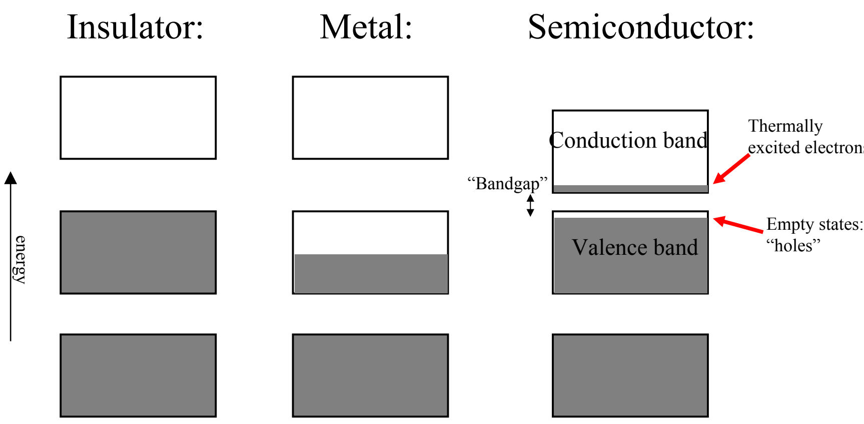
N levels -> “band” of energy

N levels -> “band” of energy

N levels -> “band” of energy

Band theory of solids:

Filled bands do not conduct electricity!



Insulator:

Metal:

Semiconductor:

Conduction band

Valence band

“Bandgap”

Thermally excited electrons

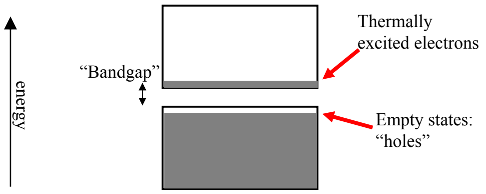
Empty states: “holes”

We usually don’t care about lower bands.

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

Semiconductors:

Finite temperature:

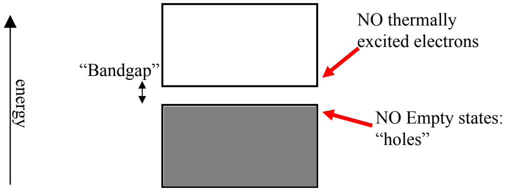


“Bandgap”

Thermally excited electrons

Empty states: “holes”

Zero temperature:



“Bandgap”

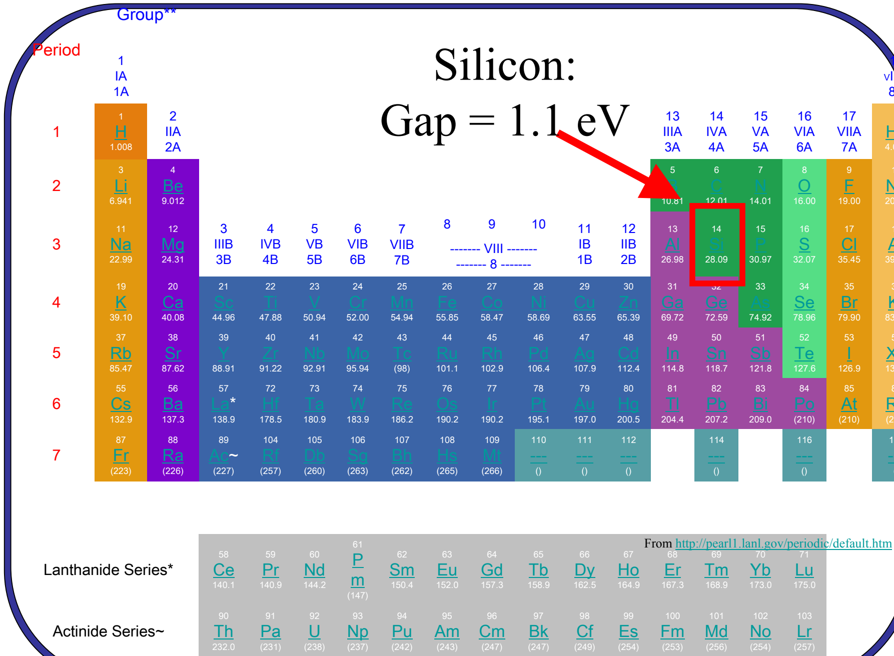
NO thermally excited electrons

NO Empty states: “holes”

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

Silicon:

Gap = 1.1 eV



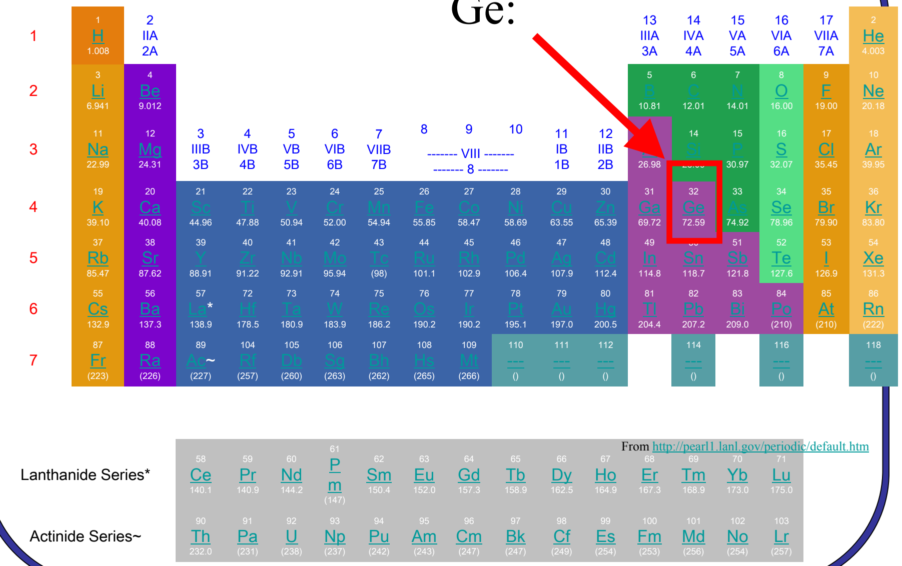
Group**

Period	1 IA 1A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 ------- VIII ------- ------- 8 -------	10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	vI 8
1	1 H 1.008																	H 4.
2	3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	N 20
3	11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	A 39
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.47	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	K 83
5	37 Rb 85.47	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	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	X 13
6	55 Cs 132.9	56 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)	R (2
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 --- ()		114 --- ()		116 --- ()		1

Lanthanide Series*	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 P m (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
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)

From http://pearl1.lanl.gov/periodic/default.htm

Ge:



Period	1 IA 1A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 ------- VIII ------- ------- 8 -------	10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	8 VIIIA 8A
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2	3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
3	11 Na 22.99	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
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.47	28 Ni 58.69	29 Cu 63.55	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
5	37 Rb 85.47	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	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	56 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)
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From http://pearl1.lanl.gov/periodic/default.htm

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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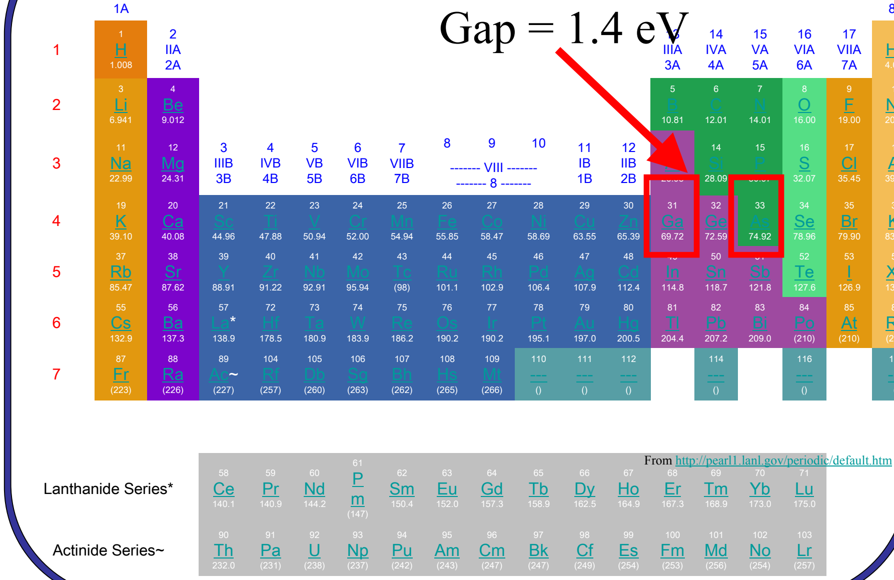
GaAs:
Gap = 1.4 eV



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4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.47	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90
5	37 Rb 85.47	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	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9
6	55 Cs 132.9	56 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)
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 --- ()		114 --- ()		116 --- ()	

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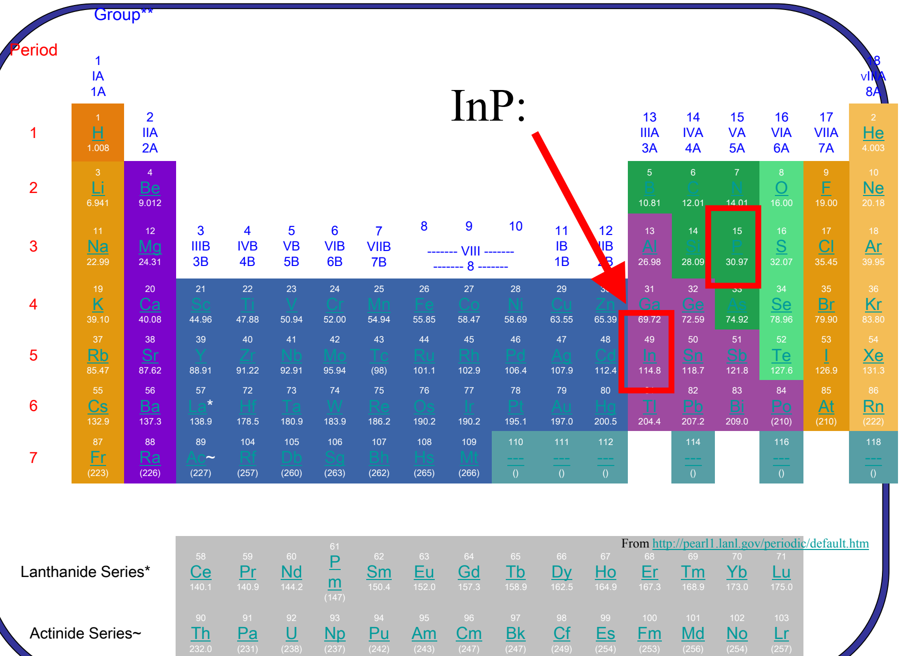
InP:



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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.

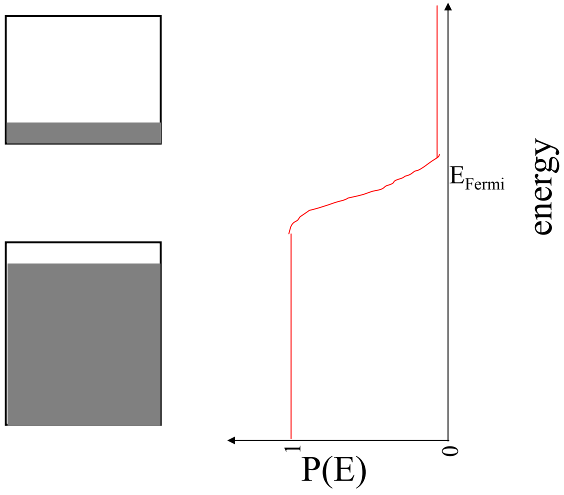
The price we pay for treating a complicated system like free electrons:

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:

Semiconductors:

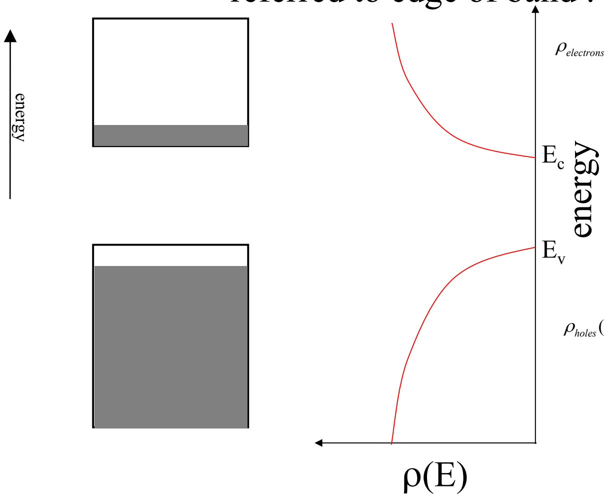
1) E_{Fermi} in middle of gap:



In board,
discuss magnitude of gap,
kT smearing.
Also high energy appr.
to Fermi-Dirac, and low
Probability of excitation!

Semiconductors:

2) Density of states origin is referred to edge of band :

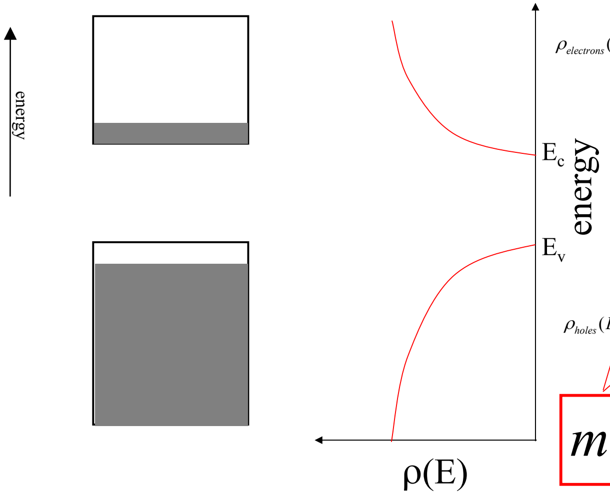


$$\rho_{electrons}(E)dE = \frac{2^{1/2}m^{3/2}}{\pi^2\hbar^{3/2}}\cdot(E-E_c)^{1/2}dE$$

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

Semiconductors:

3) Effective mass of electrons, holes:

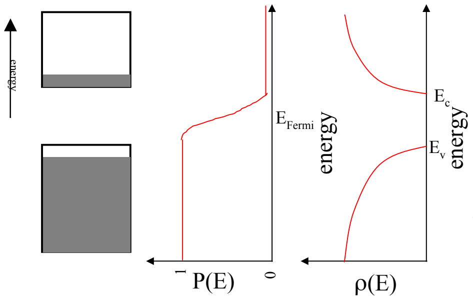


$$\rho_{electrons}(E)dE = \frac{2^{1/2}m^{3/2}}{\pi^2\hbar^{3/2}}\cdot(E-E_c)^{1/2}dE$$

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

$$\boxed{m \rightarrow m_e^*, m_h^*}$$

How many electrons in conduction band?



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

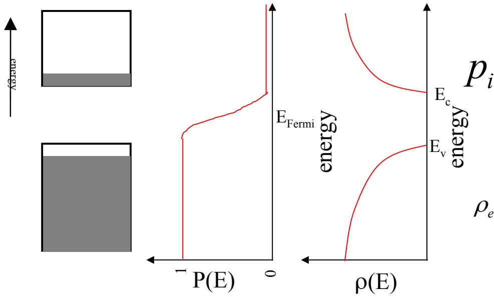
$$\rho_{electrons}(E)dE = \frac{2^{1/2}m^{3/2}}{\pi^2\hbar^{3/2}}\cdot(E-E_c)^{1/2}dE$$

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

(Discuss high energy appr. on board.)

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

How many holes in valence band?



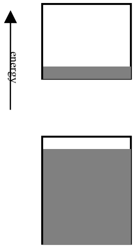
$$p_i = \int_{E_c}^{-\infty} [1-P(E)]\rho(E)dE$$

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

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

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

Holes and electrons



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

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

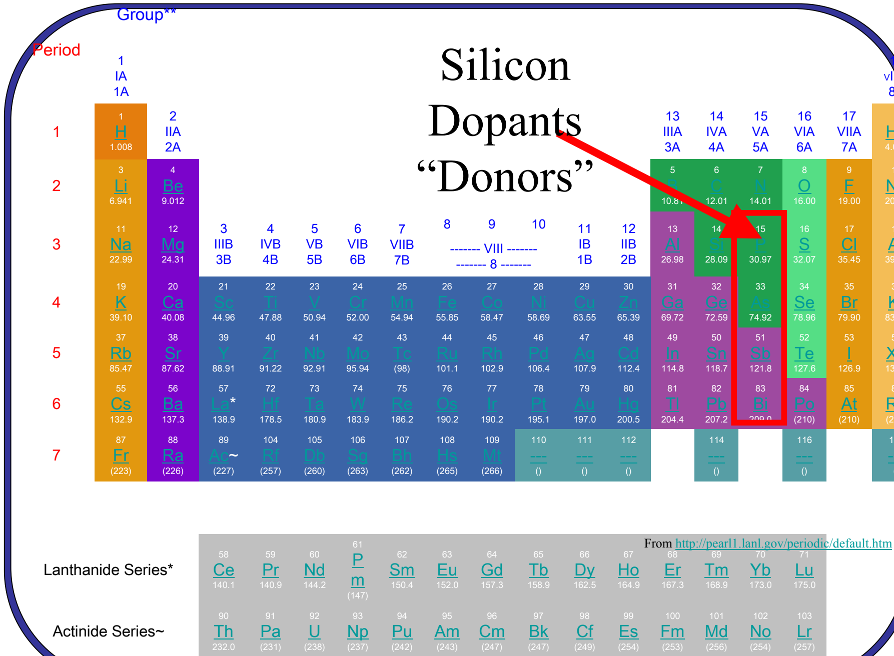
But $E_f - E_c = (1/2)\,E_{gap}$ and $E_v - E_f = (1/2)\,E_{gap}$.
With some algebra,

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

Doping

- If we purposely include some “impurities” in the crystal, we can add more electrons.
- This works if the impurity atoms have one more electron per atom than the host semiconductor.
- Since we increase # of electrons, Fermi energy increases
- Intrinsic means no doping.
- Examples discussed for Si on next slide:

Silicon Dopants “Donors”



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1	1 H 1.008																	H 4.
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5	37 Rb 85.47	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	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	X 13
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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 --- ()		114 --- ()		116 --- ()		1

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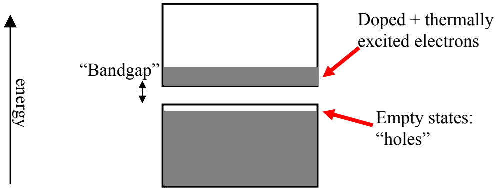
From http://pearl1.lanl.gov/periodic/default.htm

N-type doped semiconductors:

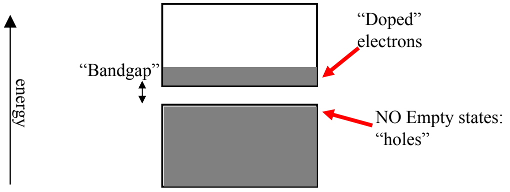
Finite temperature:



Doped + thermally excited electrons

Empty states: “holes”

“Low” temperature:

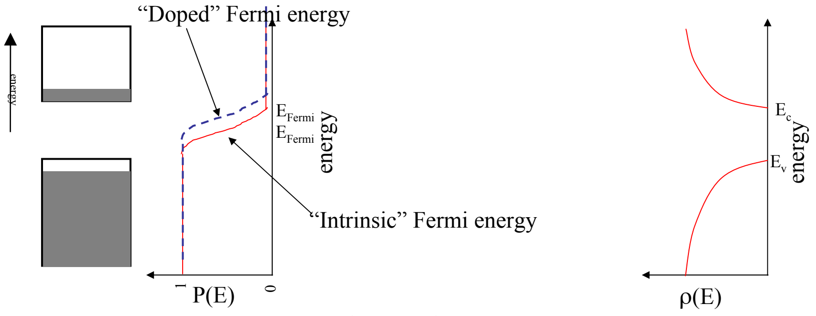


“Doped” electrons

NO Empty states: “holes”

CONDUCTION
AT LOW TEMPERATURE!

How many electrons in conduction band?



$$n_{total} = n_i + N_{donors} = 2\left(\frac{m_e^* kT}{2\pi\hbar^2}\right) e^{(E_{Fermi\,(\mathrm{intrinsic})} - E_c)/kT} + N_{donors}$$

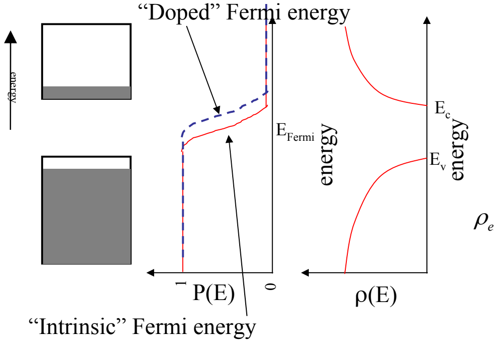
We can determine the new Fermi level by the relationship:

$$n_{total} = n_i + N_{donors} = 2\left(\frac{m_e^* kT}{2\pi\hbar^2}\right) e^{(E_{Fermi\,\mathrm{new}} - E_c)/kT}$$

HW will calculate what has to be $E_{\text{Fermi new}}$ for a given dopant density N for this formula to come out right..

How many electrons in conduction band?

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



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

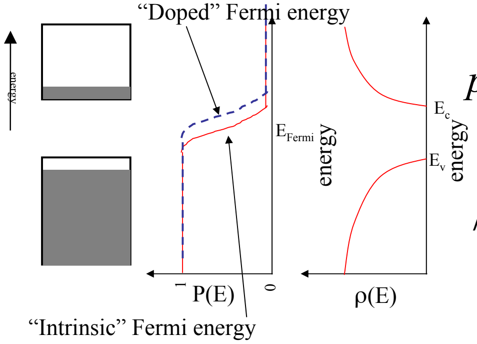
$$\rho_{electrons}(E)dE = \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^{3/2}} \cdot (E - E_c)^{1/2} dE$$

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

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

How many holes in valence band?

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



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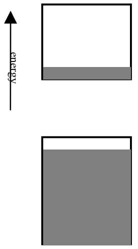
$$P(E) = \frac{1}{e^{(E - E_f)/kT} + 1}$$

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

Holes and electrons when doped N-type



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

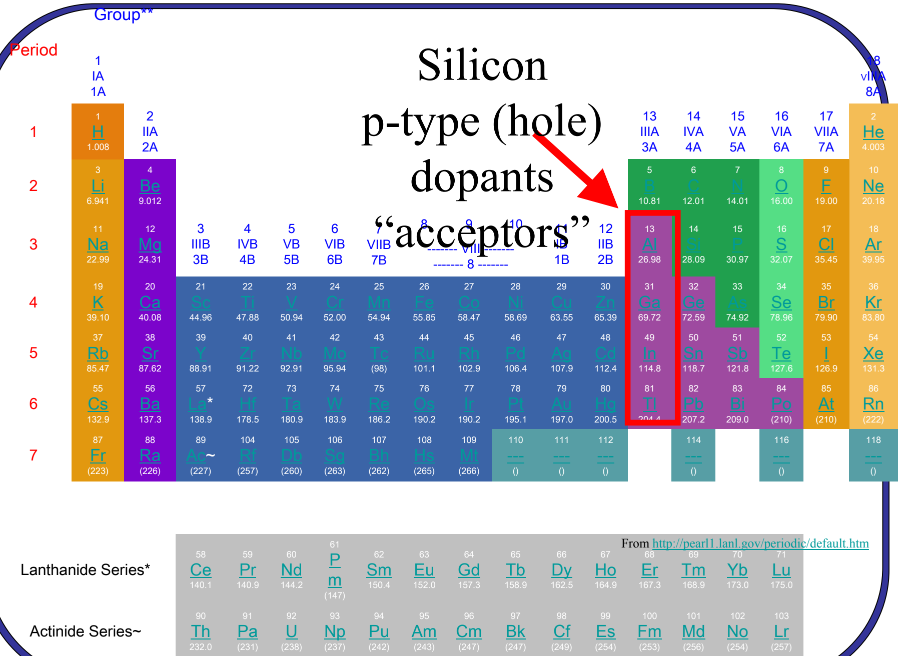
$$n = 2\left(\frac{m_e^* kT}{2\pi\hbar^2}\right)^{3/2} e^{(E_f - E_c)/kT}$$

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

$$\boxed{n > p}$$

We can do the whole exercise again with HOLES.

Silicon p-type (hole) dopants "acceptors"



Group**

Period

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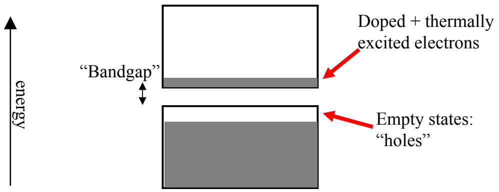
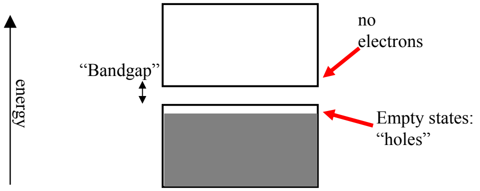
P-type doped semiconductors:

Finite temperature:

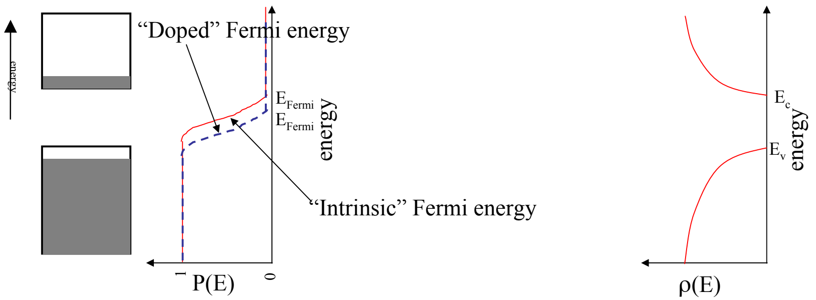


"Low" temperature:



CONDUCTION
AT LOW TEMPERATURE!

How many holes in valence band?



$$p_{total} = p_i + N_{acceptors} = 2\left(\frac{m_h^* kT}{2\pi\hbar^2}\right) e^{(E_v - E_{Fermi\,(\text{intrinsic})})/kT} + N_{acceptors}$$

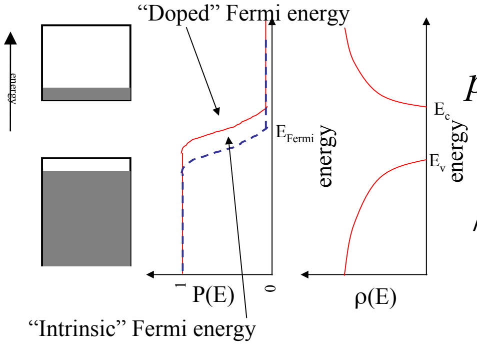
We can determine the new Fermi level by the relationship:

$$p_{total} = p_i + N_{acceptors} = 2\left(\frac{m_h^* kT}{2\pi\hbar^2}\right) e^{(E_v - E_{Fermi\ \text{new}})/kT}$$

HW will calculate what has to be $E_{\text{Fermi new}}$ for a given dopant density N for this formula to come out right..

How many holes in valence band?

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



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

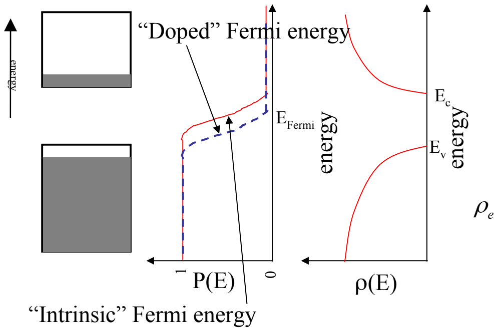
$$\rho_{electrons}(E)\,dE = \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^{3/2}} \cdot (E - E_c)^{1/2}\,dE$$

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

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

How many electrons in conduction band?

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



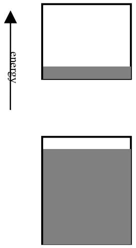
$$n_i = \int_{E_c}^{\infty} P(E)\rho(E)\,dE$$

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

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

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

Holes and electrons when doped



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

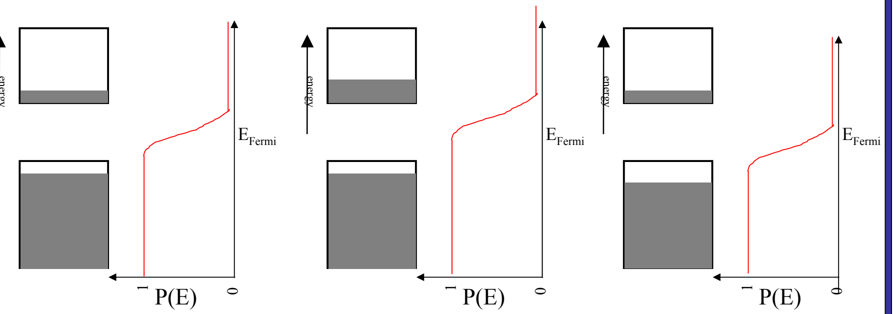
$$n = 2\left(\frac{m_e^* kT}{2\pi\hbar^2}\right)^{3/2} e^{(E_f - E_c)/kT}$$

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

$$\boxed{n < p}$$

In conclusion:

Intrinsic: n-type: p-type:



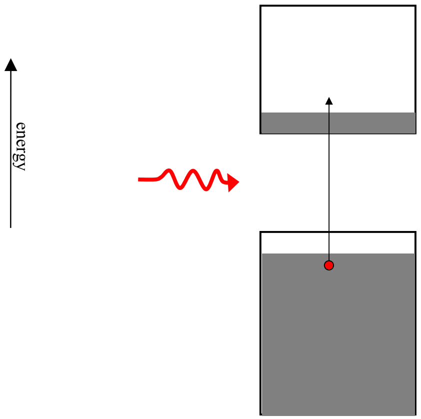
$\boxed{n = p}$ $\boxed{n > p}$ $\boxed{n < p}$

What we've done:

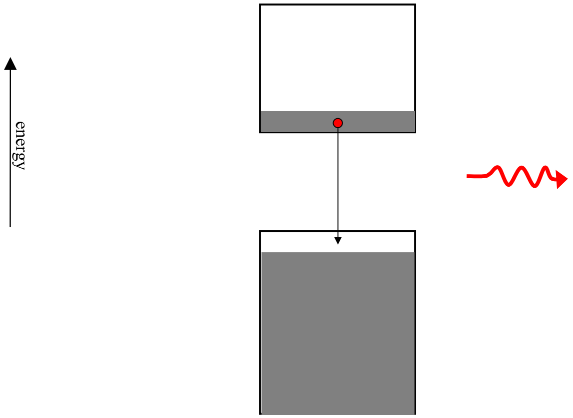
- Free electron density of states
- Fermi-Dirac distrubution function
- Band theory of solids (metal, insulator, semiconductor)
- Effective mass, density of states in semiconductors
- Electron, hole carrier concentrations in semiconductors

In future lectures:

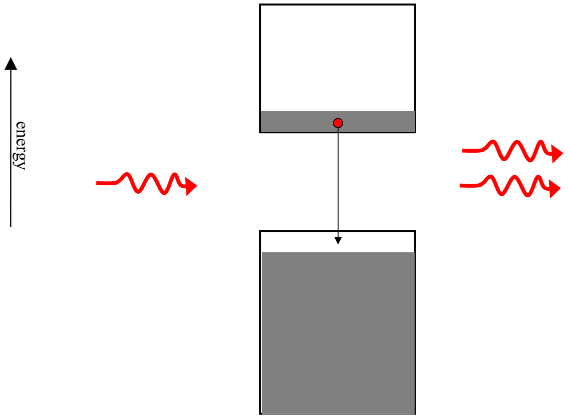
Optical transitions:
Absorption:



Optical transitions:
Spontaneous emission:



Optical transitions:
Stimulated emission:



Why can’t this lase?