ECE606: Solid State Devices
Lecture 6

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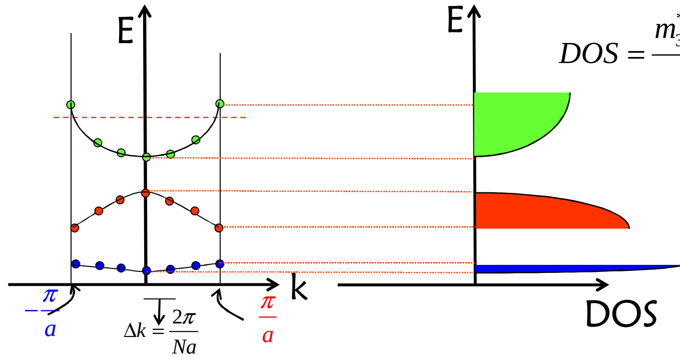
Presentation Outline

- Reminder – Density of states
  - »Possible states as a function of Energy
- Reality check - Measurements of Bandgaps
- Reality check - Measurements of Effective Mass
- Rules of filling electronic states
- Derivation of Fermi-Dirac Statistics: three techniques
- Intrinsic carrier concentration
- Conclusions

Reference: Vol. 6, Ch. 3 & 4

Reminder: Momentum vs. DOS

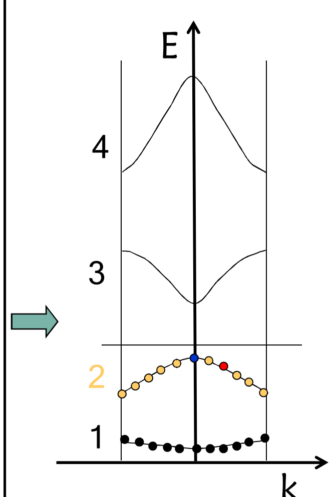


$$DOS = \frac{m_3^* \sqrt{2m_3^* (E - E_0)}}{\pi^2 \hbar^3}$$

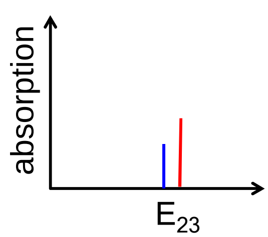
Important things to remember:

- Momentum k entered our thinking as a quantum number
- Each quantum number is creating ONE state
- Often "just" need the number of available states in an energy range
  => Density of States
  => appears to be solely determined by
  - » 1) band edge,
  - » 2) effective mass

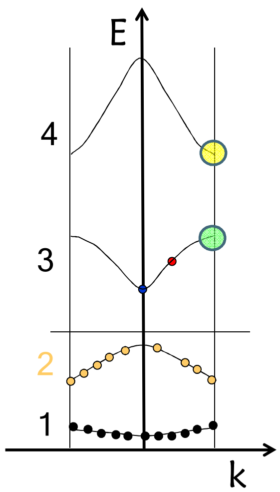
Measurement of Band Gap

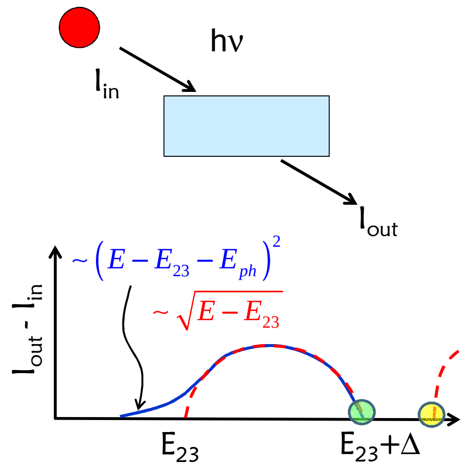


Photons are only absorbed between bands that have filled and empty states

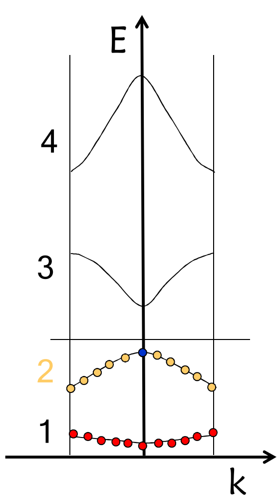


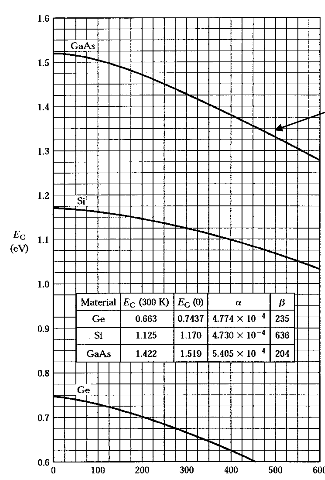
Measurement of Energy Gap





Temperature-dependent Band Gap





Material	E_G (300 K)	E_G (0)	α	β
Ge	0.663	0.7437	4.774×10^{-4}	235
Si	1.125	1.170	4.730×10^{-4}	636
GaAs	1.422	1.519	5.405×10^{-4}	204

$$E_G(T) = E_G(0) - \frac{\alpha T^2}{T + \beta}$$

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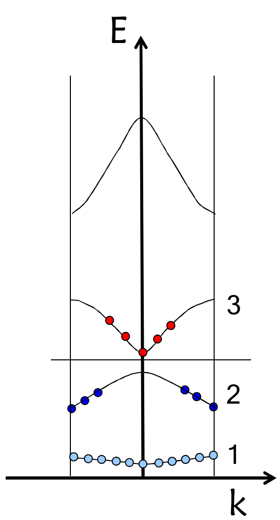
Measurements of Effective Masses



Important things to remember:
- Full bands do not conduct – electrons have no space to go
- Empty bands to not conduct – there are no electrons to go around

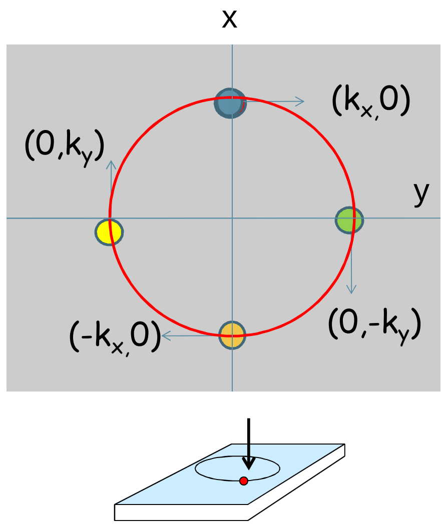
Question:
- We are interested in the top-most valence band holes and the bottom-most electron states
- We want to figure out the slope of the bands
- How can we probe just one particular species of electrons/holes?
- We do not want to transfer them from one band to the next!

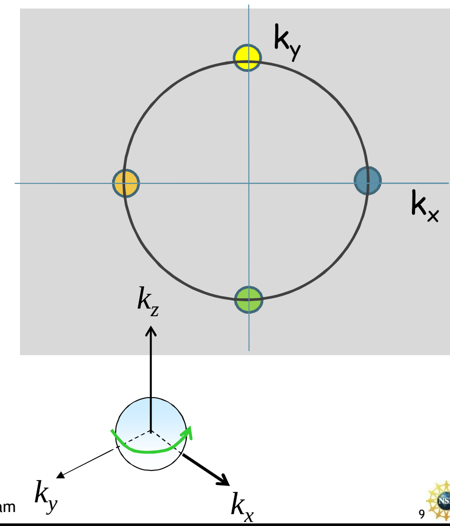
=> can we rotate the electrons around in a single band?

Motion in Real Space and Phase Space

Energy=constant.

Liquid He temperature …





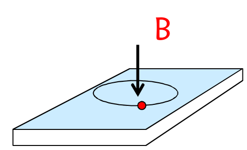
Derive the Cyclotron Formula

$$m^* = \frac{qB_0}{2\pi \nu_0}$$

For an particle in (x-y) plane with B-field in z-direction, the Lorentz force is …

$$\frac{m^* \upsilon^2}{r_0} = q\upsilon \times B_z = q\upsilon B_z$$

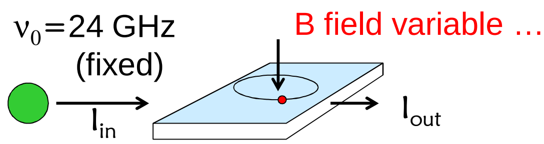
$$\upsilon = \frac{qB_0 r_0}{m^*}$$

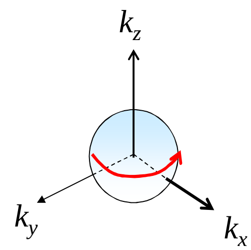


$$\tau = \frac{2\pi r_0}{\upsilon} = \frac{2\pi m^*}{qB_0}$$

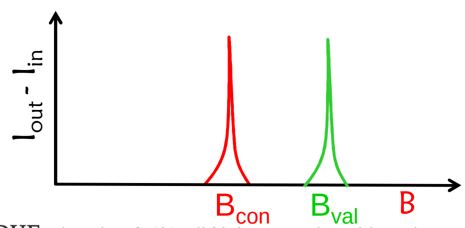
$$\nu_0 \equiv \frac{1}{\tau} = \frac{qB_0}{2\pi m^*}$$

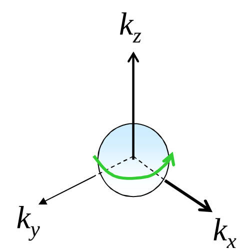
$$\omega_0 = 2\pi \nu_0 = \frac{qB_0}{m^*}$$

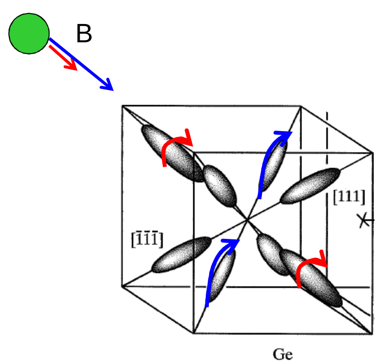




$$\nu_0 = \frac{qB_0}{2\pi m^*} \qquad m^* = \frac{qB_0}{2\pi \nu_0}$$







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$[1\bar{1}\bar{1}]$ $[1\bar{1}\bar{1}]$ $[\bar{1}1\bar{1}]$ $[111]$

4 angles between B field and the ellipsoids …
Recall the HW1

Show that $$\frac{1}{m_c^{\,2}} = \frac{\cos^2\theta}{m_t^{\,2}} + \frac{\sin^2\theta}{m_l m_t}$$

Given three m_c and three θ, we will Find m_t, and m_l

The Lorentz force on electrons in a B-field

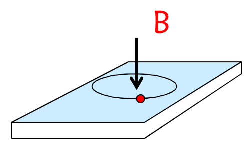
$$F = q\upsilon \times B = [M]\frac{d\upsilon}{dt}$$

In other words,

$$F_x = q(\upsilon_y B_z - \upsilon_z B_y) = m_t^* \frac{d\upsilon_x}{dt}$$

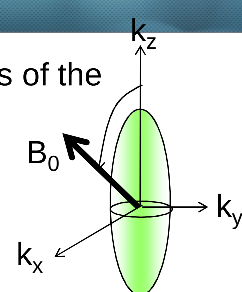
$$F_y = q(\upsilon_z B_x - \upsilon_x B_z) = m_t^* \frac{d\upsilon_y}{dt}$$

$$F_z = q(\upsilon_x B_y - \upsilon_y B_x) = m_l^* \frac{d\upsilon_z}{dt}$$



Let (B) make an angle (θ) with longitudinal axis of the ellipsoid (ellipsoids oriented along k_z)

$$B_x = B_0 \cos(\theta),\; B_y = 0,\; B_z = B_0 \sin(\theta),$$



Differentiate (v_y) and use other equations to find …

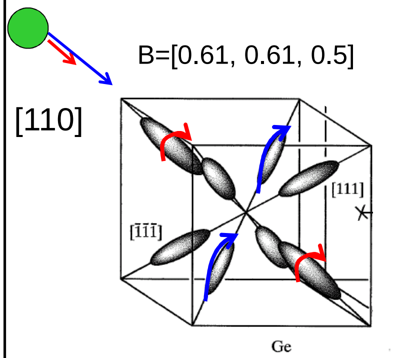
$$\frac{d^2\upsilon_y}{dt^2} + \upsilon_y \omega^2 = 0 \quad \text{with} \quad \omega^2 \equiv \left[\omega_t w_l \sin^2\theta + \omega_t^{\,2}\cos^2\theta\right]$$

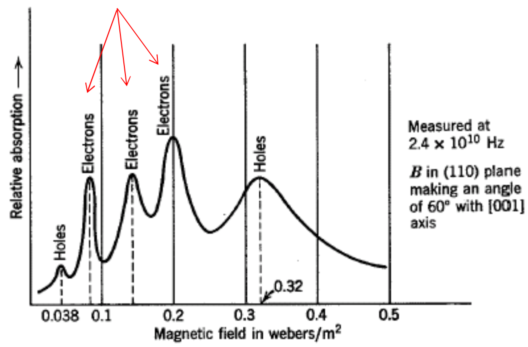
$$\omega_0 \equiv \frac{qB_0}{m_c^*} \qquad \omega_t \equiv \frac{qB_0}{m_t^*} \qquad \omega_l \equiv \frac{qB_0}{m_l^*}$$

so that … $$\frac{1}{(m_c^*)^2} = \frac{\sin^2\theta}{m_l m_t} + \frac{\cos^2\theta}{m_t^{\,2}}$$

B=[0.61, 0.61, 0.5]

[110]



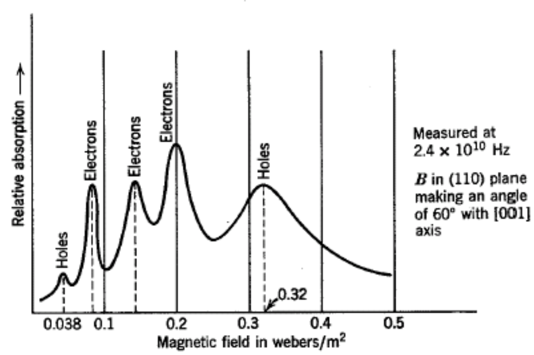


$$\frac{1}{m_c^2} = \frac{\cos^2\theta}{m_t^2} + \frac{\sin^2\theta}{m_l m_t}$$

Three peaks B_1, B_2, B_3
Three masses m_{c1}, m_{c2}, m_{c3}
Three unique angles: 7, 65, 73

$$m_c = \frac{qB_1}{2\pi\nu_0}$$

Known θ and m_c allows calculation of m_t and m_l.



Which peaks relate to valence band?
Why are there two valence band peaks?

Conclusions

1) Only a fraction of the available states are occupied. The number of available states change with energy. DOS captures this variation.
2) DOS is an important and useful characteristic of a material that should be understood carefully.
3) Experimental measurements are key to making sure that the theoretical calculations are correct. We will discuss them in the next class.

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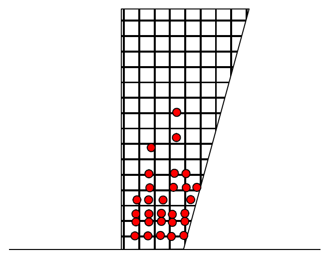
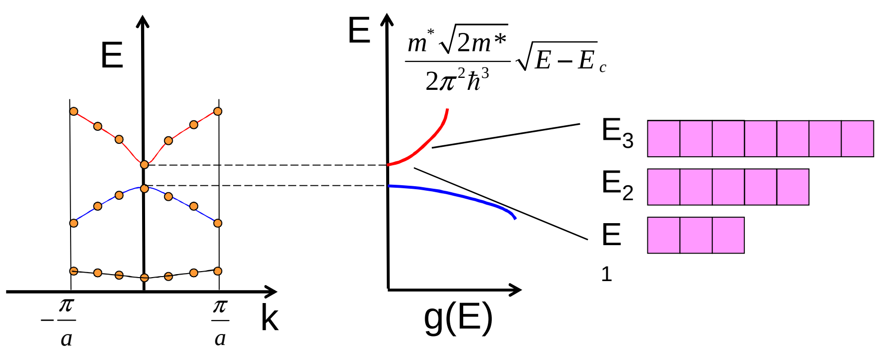
Carrier number = Number of states x ***filling factor***

Chapters 2-3 Chapter 4

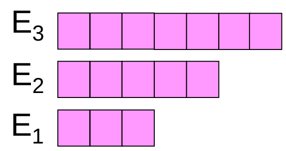


Energy-Band

Density of States



Rules for filling up the States



- Pauli Principle: Only one electron per state
- Total number of electrons is conserved $N_T = \sum_i N_i$
- Total energy of the system is conserved $E_T = \sum_i E_i N_i$

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In 1926, Fowler studied collapse of a star to white dwarf by F-D statistics, before Sommerfeld used the F-D statistics to develop a theory of electrons in metals in 1927. Wikipedia has a nice article on this topic.

Diff. between a trick and a method:
A method is a trick used more than once!

Illustrative Example: 3 Energy Levels

Particle conservation

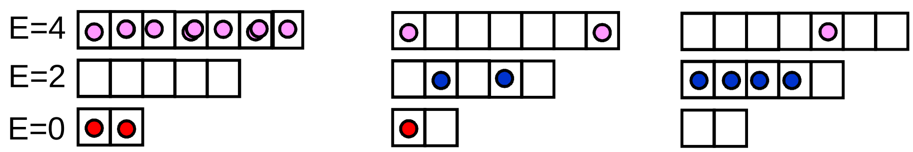
$$N_T = \sum_i N_i$$

N_T=5

Energy conservation

$$E_T = \sum_i E_i N_i$$

E_T=12

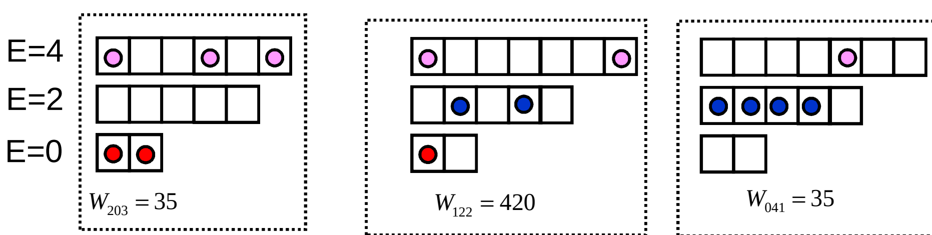


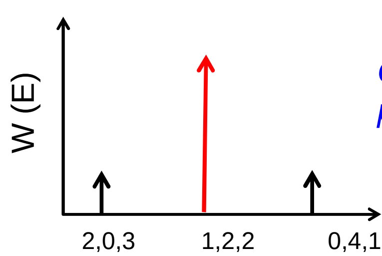
$$W_{203} = \frac{2!}{1!2!} \bullet \frac{5!}{0!5!} \bullet \frac{7!}{3!4!} = 35$$

$$W_{122} = \frac{2!}{1!1!} \bullet \frac{5!}{2!3!} \bullet \frac{7!}{5!2!} = 420$$

$$W_{041} = \frac{2!}{0!2!} \bullet \frac{5!}{4!1!} \bullet \frac{7!}{6!1!} = 35$$

Occupation Statistics



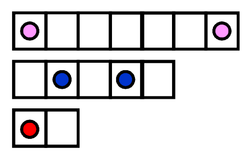


Choose the most probable configuration.

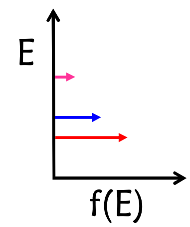
E=4 $\quad f_3^* = \frac{2}{7}$

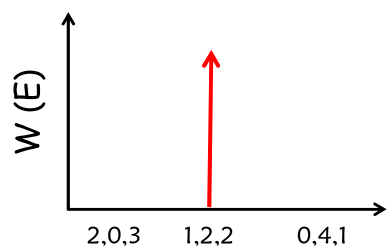
E=2 $\quad f_2^* = \frac{2}{5}$

E=0 $\quad f_1^* = \frac{1}{2}$



$W_{122} = 420$

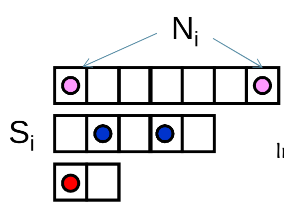


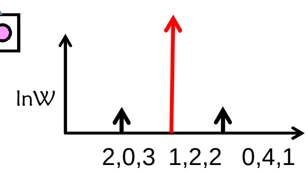


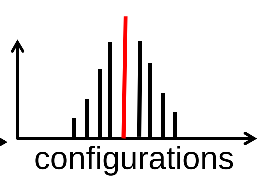
Side note:
So far everything shown here is EXACT!
No approximations on the occupation probability!
=> direct application to nano-scale electronics!

Stirling approx.

$\ln(S!) \approx S\ln(S) - S \quad for \;\; S > 10$







$$W_c = \prod_i \frac{S_i!}{(S_i - N_i)!N_i!}$$

Recall. $W_{203} = \frac{2!}{1!2!} \bullet \frac{5!}{0!5!} \bullet \frac{7!}{3!4!}$

$$\ln(W) = \sum_i [\ln S_i! - \ln(S_i - N_i)! - \ln N_i!]$$

$$\simeq \sum_i [S_i \ln S_i - S_i - (S_i - N_i)\ln(S_i - N_i) + (S_i - N_i) - N_i \ln N_i + N_i]$$

$$= \sum_i [S_i \ln S_i - (S_i - N_i)\ln(S_i - N_i) - N_i \ln N_i]$$

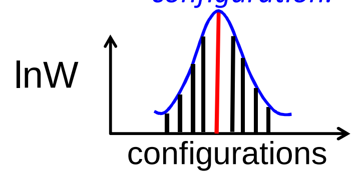
Optimization with Lagrange-Multiplier

Choose the most probable configuration.

$$\ln W = \sum_i \left[S_i \ln S_i - (S_i - N_i)\ln(S_i - N_i) - N_i \ln N_i \right]$$

$$\delta \ln(W) = \sum_i \frac{\partial \ln W}{\partial N_i} dN_i$$

$$= \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1 \right) dN_i \right]$$



Optimization with constraints!

$$\simeq \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1 \right) dN_i \right] - \alpha \sum_i dN_i - \beta \sum_i E_i dN_i$$

Energy conservation $E_T = \sum_i E_i N_i$

$$= \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1 \right) - \alpha - \beta E_i \right] dN_i$$

$$= 0$$

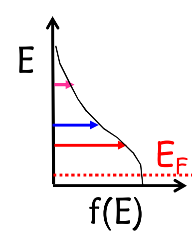
$N_T = \sum_i N_i$ *Particle conservation*

See additional notes on Lagrange multiplies on ece606 page and blackboard

Final steps …

$$\delta \ln W = \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1 \right) - \alpha - \beta E_i \right] dN_i = 0$$

$$\left[\ln\left(\frac{S_i}{N_i} - 1 \right) - \alpha - \beta E_i \right] = 0$$



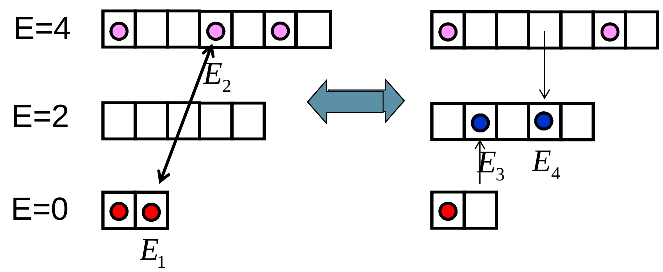
$$f(E) \equiv \frac{N_i}{S_i} = \frac{1}{1 + e^{\alpha + \beta E}} \qquad f_{\max}(E) = 1$$

$$\text{At } E = E_F, \; f(E_F) \equiv \frac{1}{2} \quad \Rightarrow \alpha + \beta E_F = 0$$

$$f(E) = \frac{N_i}{S_i} = \frac{1}{1 + e^{\beta(E - E_F)}} \qquad = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

$$\text{At } E \to \infty, \; f_{Boltzman}(E) = A e^{-E/k_B T} \quad \Rightarrow \quad \beta = \frac{1}{k_B T}$$

Derivation by Detailed Balance



Detailed Balance in Equilibrium

$$f_0(E_1)\,f_0(E_2)[1-f_0(E_3)][1-f_0(E_4)]$$ ⇨ Pauli Exclusion

⇦ $$= f_0(E_3)\,f_0(E_4)[1-f_0(E_1)][1-f_0(E_2)]$$

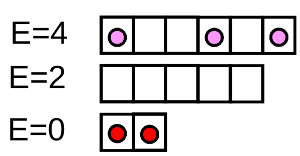
Energy conversation

$$E_1 + E_2 = E_3 + E_4$$

Only solution is … $f_0(E) = \dfrac{1}{1+e^{\beta(E-E_F)}}$

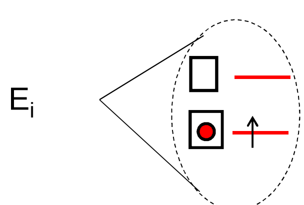
- Pauli Principle, energy, and number conservation all satisfied

Derivation by Partition Function



$$P_i = \frac{e^{-\beta(E_i - N_i E_F)}}{\sum_i e^{-\beta(E_i - N_i E_F)}} \equiv \frac{e^{-\beta(E_i - N_i E_F)}}{Z}$$

$$\beta = 1/k_B T$$



$state$	E_i	N_i	P_i
0	0	0	$e^{-\beta(0-0\times E_F)}/Z$
1	1	1	$e^{-\beta(E_i-1\times E_F)}/Z$

Derivation by Partition Function

1

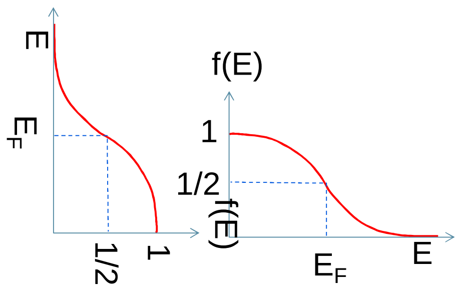
$state$	E_i	N_i	P_i
0	0	0	$e^{-\beta(0-0\times E_F)}/Z$
1	1	1	$e^{-\beta(E_i-1\times E_F)}/Z$

Probability that state is filled …

$$f(E)=\frac{P_1}{P_0+P_1}$$

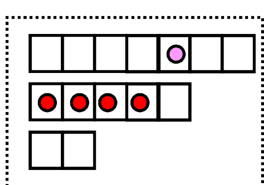
$$=\frac{e^{-(E_i-E_F)/k_BT}/Z}{1/Z+e^{-(E_i-E_F)/k_BT}/Z}$$

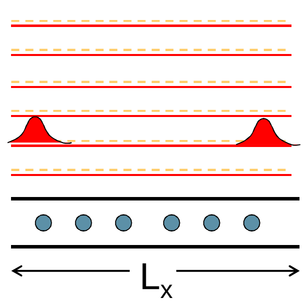
$$=\frac{1}{1+e^{(E_i-E_F)/k_BT}}$$



Few comments on Fermi-Dirac Statistics

- Applies to all spin-1/2 particles
- Information about spin is not explicit; multiply DOS by 2. May be more complicated for magnetic semiconductors.
- Coulomb-interaction among particles is neglected, Therefore it applies to extended solids, not to small molecule

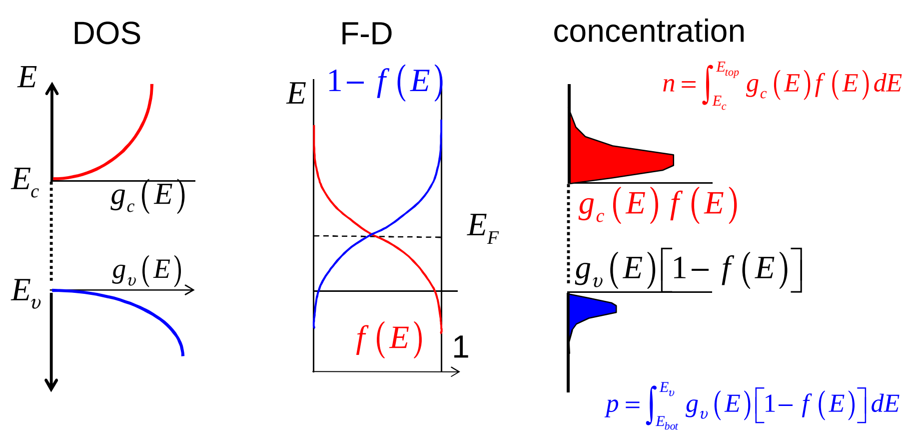




Presentation Outline

- Reminder – Density of states
  - »Possible states as a function of Energy
- Reality check - Measurements of Bandgaps
- Reality check - Measurements of Effective Mass
- Rules of filling electronic states
- Derivation of Fermi-Dirac Statistics: three techniques
- Intrinsic carrier concentration
- Conclusions

Carrier Distribution



$$n = \int_{E_c}^{E_{top}} g_c(E) f(E)\, dE$$

$$= \int_{E_c}^{E_{top}} 2 \times \frac{m_n^* \sqrt{2 m_n^* (E - E_C)}}{2\pi^2 \hbar^3} \frac{1}{1 + e^{\beta(E - E_F)}}\, dE$$

Include spin factor of 2

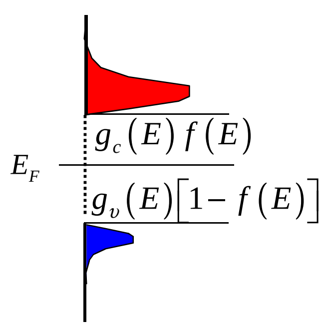
$$\simeq \int_{E_c}^{\infty} \frac{m_n^* \sqrt{2 m_n^* (E - E_C)}}{\pi^2 \hbar^3} \frac{1}{1 + e^{\beta(E - E_c)} e^{\beta(E_c - E_F)}}\, dE$$

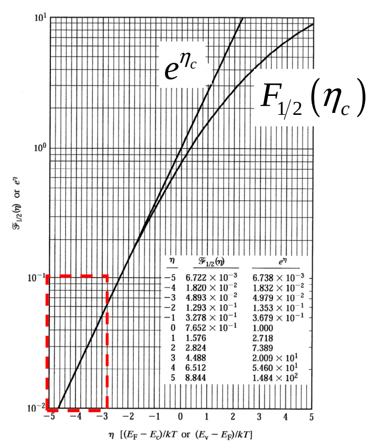
Assume wide bands

$$= N_C \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_c) \qquad \eta_c \equiv \beta(E_F - E_C)$$

$$N_C \equiv 2\left(\frac{2\pi m_n^* \beta}{h^2}\right)^{3/2} \qquad F_{1/2}(\eta) = \int_0^{\infty} \frac{\sqrt{\xi}\, d\xi}{1 + e^{\xi - \eta}}$$

$$n = N_C \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_c) \to N_C e^{\eta_c} \quad if \quad -\eta_c \equiv \beta(E_C - E_F) > 3$$





η	$\mathscr{F}_{1/2}(\eta)$	e^{η}
−5	6.722×10^{-3}	6.738×10^{-3}
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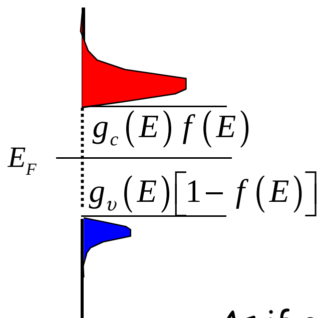
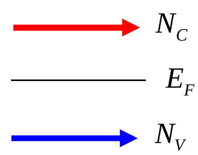
Effective Density of States

$$n = N_C \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_c) \to N_C e^{-\beta(E_c - E_F)} \quad if \quad E_c - E_F > 3\beta$$





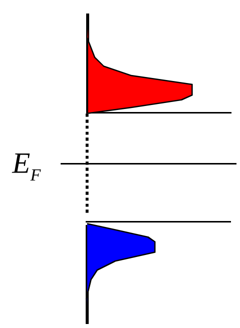
As if all states are at a single level E_C

Law of Mass-Action

$$n = N_C e^{-\beta(E_c - E_F)}$$

$$p = N_V e^{+\beta(E_v - E_F)}$$

$$n \times p = N_C N_V e^{-\beta(E_c - E_v)}$$
$$= N_C N_V e^{-\beta E_g}$$



Product is independent of the Fermi level!
Very useful balance equation! Will use it often

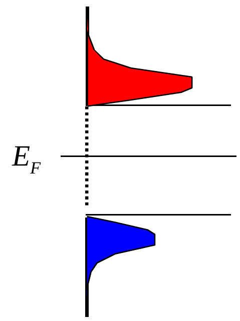
Fermi-Level for Intrinsic Semiconductors

$$n = p = n_i$$

$$n_i^2 = N_C N_V e^{-\beta E_g}$$

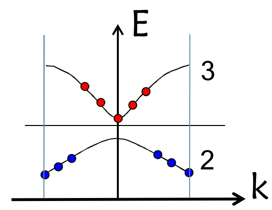
$$n_i = \sqrt{N_C N_V} e^{-\beta E_g/2}$$

$$E_F \equiv E_i$$



$$n = p \Rightarrow N_C e^{-\beta(E_c - E_i)} = N_V e^{+\beta(E_v - E_i)}$$

$$E_i = \frac{E_G}{2} + \frac{1}{2\beta} ln \frac{N_V}{N_C}$$



Conclusions

- We discussed how electrons are distributed in electronic states defined by the solution of Schrodinger equation.
- Since electrons are distributed according to their energy, irrespective of their momentum states, the previously developed concepts of constant energy surfaces, density of states etc. turn out to be very useful.
  => will not discuss Schroedinger Eq. anymore
  => everything is captured in bandedges and effective masses
- We still do not know where E_F is for general semiconductors … If we did, we could calculate electron concentration.

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Illustrative Example: 3 Energy Levels

Particle conservation

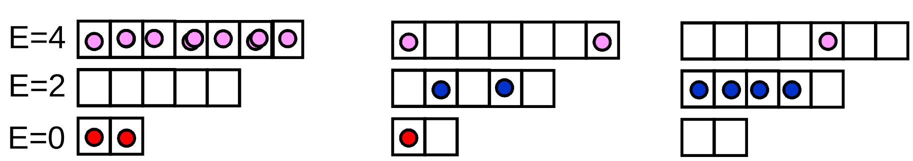
$$N_T = \sum_i N_i$$

N_T=5

Energy conservation

$$E_T = \sum_i E_i N_i$$

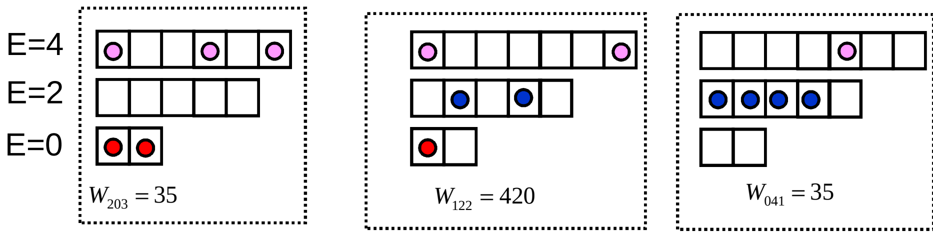
E_T=12

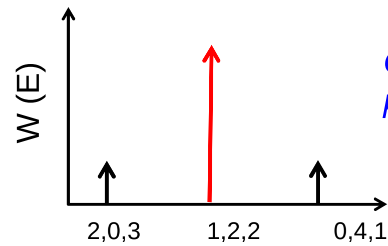


$$W_{203} = \frac{2!}{1!2!} \bullet \frac{5!}{0!5!} \bullet \frac{7!}{3!4!} = 35$$

$$W_{122} = \frac{2!}{1!1!} \bullet \frac{5!}{2!3!} \bullet \frac{7!}{5!2!} = 420$$

$$W_{041} = \frac{2!}{0!2!} \bullet \frac{5!}{4!1!} \bullet \frac{7!}{6!1!} = 35$$



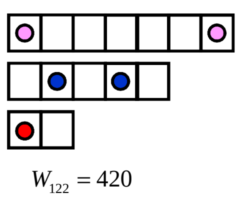


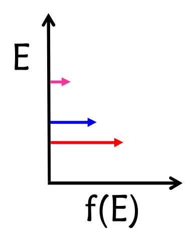
Choose the most probable configuration.

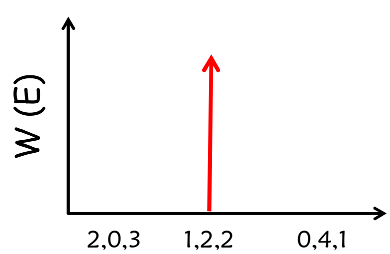
E=4 $f_3^* = \frac{2}{7}$

E=2 $f_2^* = \frac{2}{5}$

E=0 $f_1^* = \frac{1}{2}$





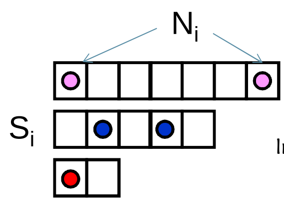


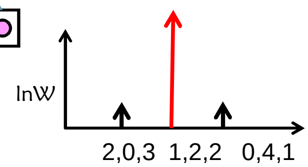
Side note:
So far everything shown here is EXACT!
No approximations on the occupation probability!
=> direct application to nano-scale electronics!

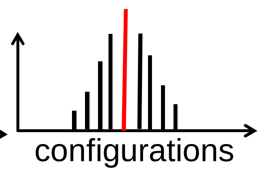
For N-states

Stirling approx.

$\ln(S!) \approx S\ln(S) - S \quad for \;\; S > 10$







$$W_c = \prod_i \frac{S_i!}{(S_i - N_i)!N_i!}$$

Recall. $W_{203} = \frac{2!}{1!2!} \bullet \frac{5!}{0!5!} \bullet \frac{7!}{3!4!}$

$$\ln(W) = \sum_i [\ln S_i! - \ln(S_i - N_i)! - \ln N_i!]$$

$$\simeq \sum_i [S_i \ln S_i - S_i - (S_i - N_i)\ln(S_i - N_i) + (S_i - N_i) - N_i \ln N_i + N_i]$$

$$= \sum_i [S_i \ln S_i - (S_i - N_i)\ln(S_i - N_i) - N_i \ln N_i]$$

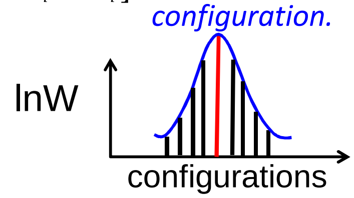
Optimization with Lagrange-Multiplier

Choose the most probable configuration.

$$\ln W = \sum_i [S_i \ln S_i - (S_i - N_i)\ln(S_i - N_i) - N_i \ln N_i]$$

$$\delta \ln(W) = \sum_i \frac{\partial \ln W}{\partial N_i} dN_i$$

$$= \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1\right) dN_i \right]$$



Optimization with constraints!

$$\simeq \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1\right) dN_i \right] - \alpha \sum_i dN_i - \beta \sum_i E_i dN_i$$

$$= \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1\right) - \alpha - \beta E_i \right] dN_i$$

$$= 0$$

Energy conservation $E_T = \sum_i E_i N_i$

$N_T = \sum_i N_i$ *Particle conservation*

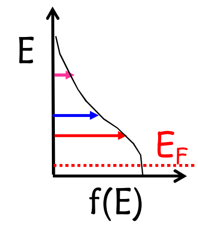
See additional notes on Lagrange multipliers on ece606 page and blackboard

Final steps …

$$\delta \ln W = \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1 \right) - \alpha - \beta E_i \right] dN_i = 0$$

$$\left[\ln\left(\frac{S_i}{N_i} - 1 \right) - \alpha - \beta E_i \right] = 0$$

$$f(E) \equiv \frac{N_i}{S_i} = \frac{1}{1 + e^{\alpha + \beta E}} \qquad f_{max}(E) = 1$$



$$\text{At } E = E_F, \ f(E_F) \equiv \frac{1}{2} \quad \Rightarrow \alpha + \beta E_F = 0$$

$$f(E) = \frac{N_i}{S_i} = \frac{1}{1 + e^{\beta(E - E_F)}} = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

$$\text{At } E \to \infty, \ f_{Boltzman}(E) = A e^{-E/k_B T} \quad \Rightarrow \quad \beta = \frac{1}{k_B T}$$

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- Potential, field, and charge
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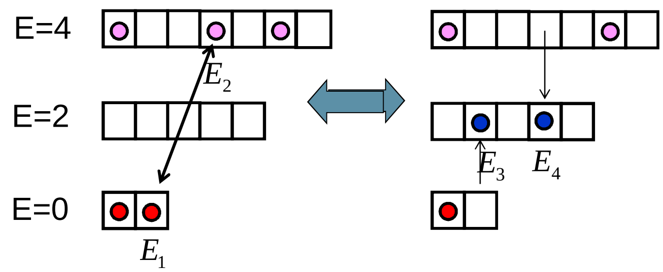
- Basic concepts of donors and acceptors
- Conclusions

Reference: Vol. 6, Ch. 3 & 4

Derivation by Detailed Balance



Detailed Balance in Equilibrium

$$f_0(E_1)\, f_0(E_2)[1-f_0(E_3)][1-f_0(E_4)]$$

Pauli Exclusion

$$= f_0(E_3)\, f_0(E_4)[1-f_0(E_1)][1-f_0(E_2)]$$

Energy conversation

$$E_1 + E_2 = E_3 + E_4$$

Only solution is … $f_0(E) = \dfrac{1}{1+e^{\beta(E-E_F)}}$

- Pauli Principle, energy, and number conservation all satisfied

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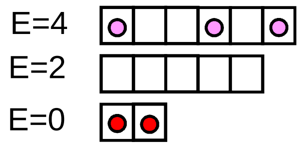
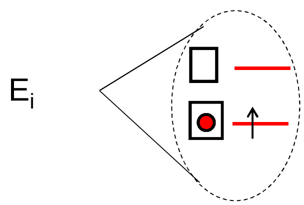


$$P_i = \frac{e^{-\beta(E_i - N_i E_F)}}{\sum_i e^{-\beta(E_i - N_i E_F)}} \equiv \frac{e^{-\beta(E_i - N_i E_F)}}{Z}$$

$$\beta = 1/k_B T$$



state	E_i	N_i	P_i
0	0	0	$e^{-\beta(0-0\times E_F)}/Z$
1	1	1	$e^{-\beta(E_i-1\times E_F)}/Z$

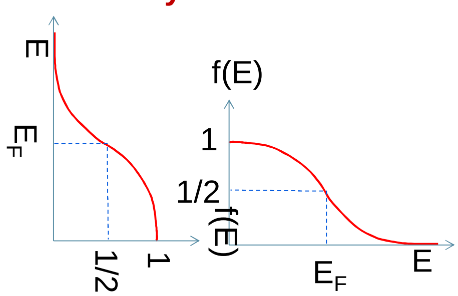
state	E_i	N_i	P_i
0	0	0	$e^{-\beta(0-0\times E_F)}/Z$ (1)
1	1	1	$e^{-\beta(E_i-1\times E_F)}/Z$

Probability that state is filled ...

$$f(E) = \frac{P_1}{P_0 + P_1}$$

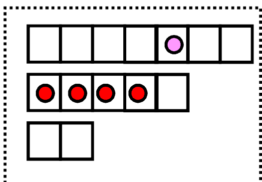
$$= \frac{e^{-(E_i - E_F)/k_B T} / Z}{1/Z + e^{-(E_i - E_F)/k_B T}/Z}$$

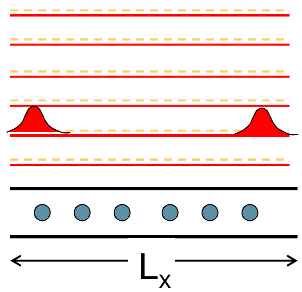
$$= \frac{1}{1 + e^{(E_i - E_F)/k_B T}}$$



Few comments on Fermi-Dirac Statistics

- Applies to all spin-1/2 particles
- Information about spin is not explicit; multiply DOS by 2. May be more complicated for magnetic semiconductors.
- Coulomb-interaction among particles is neglected, Therefore it applies to extended solids, not to small molecule





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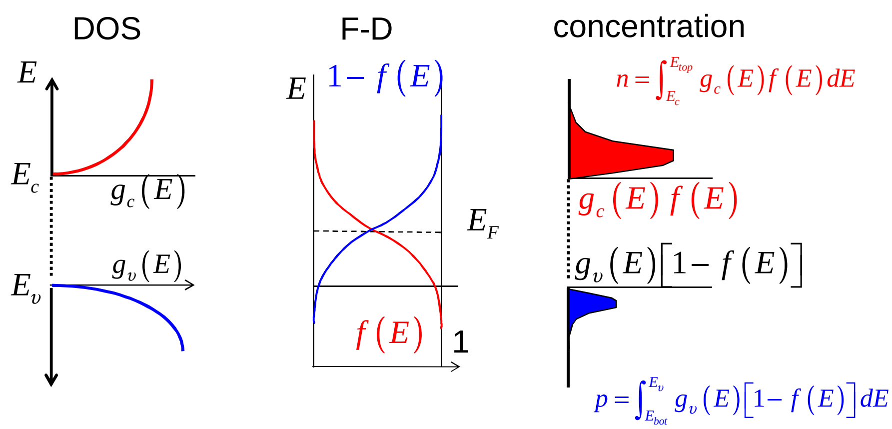

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Include spin factor of 2

$$\simeq\int_{E_c}^{\infty}\frac{m_n^*\sqrt{2m_n^*(E-E_C)}}{\pi^2\hbar^3}\frac{1}{1+e^{\beta(E-E_c)}e^{\beta(E_c-E_F)}}dE$$

Assume wide bands

$$=N_C\frac{2}{\sqrt{\pi}}F_{1/2}(\eta_c)\qquad \eta_c\equiv\beta(E_F-E_C)$$

$$N_C\equiv 2\left(\frac{2\pi m_n^*\beta}{h^2}\right)^{3/2}\qquad F_{1/2}(\eta)=\int_0^\infty\frac{\sqrt{\xi}d\xi}{1+e^{\xi-\eta}}$$

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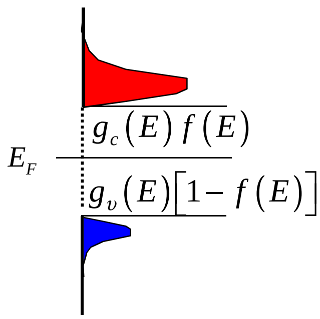

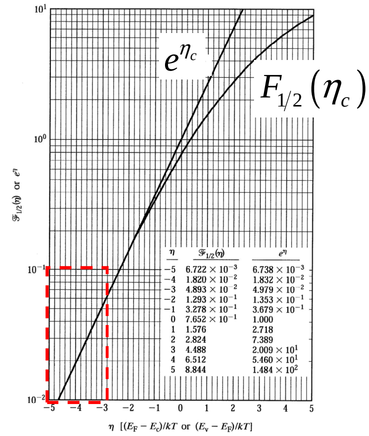

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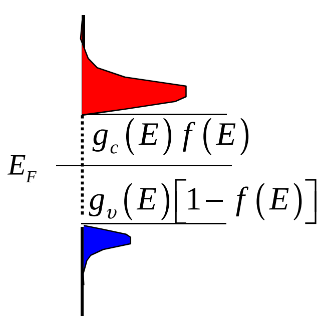

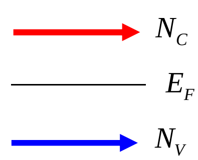

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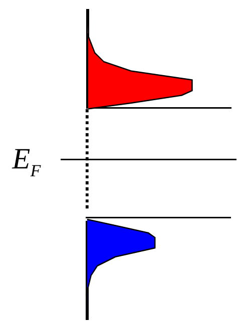

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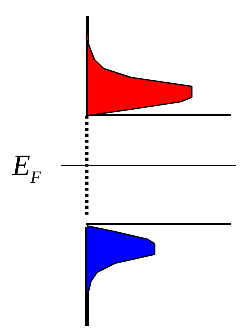
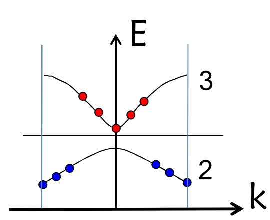


$$n = p \Rightarrow N_C e^{-\beta(E_c - E_i)} = N_V e^{+\beta(E_v - E_i)}$$

$$E_i = \frac{E_G}{2} + \frac{1}{2\beta} ln \frac{N_V}{N_C}$$



Summary - DOS and Fermi Functions

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Presentation Outline

- Schrodinger equation in periodic U(x)
- Bloch theorem
- Band structure
- Properties of electronic bands
- E-k diagram and constant energy surfaces
- Conclusions

Reference: Vol. 6, Ch. 3