

EE-606: Solid State Devices

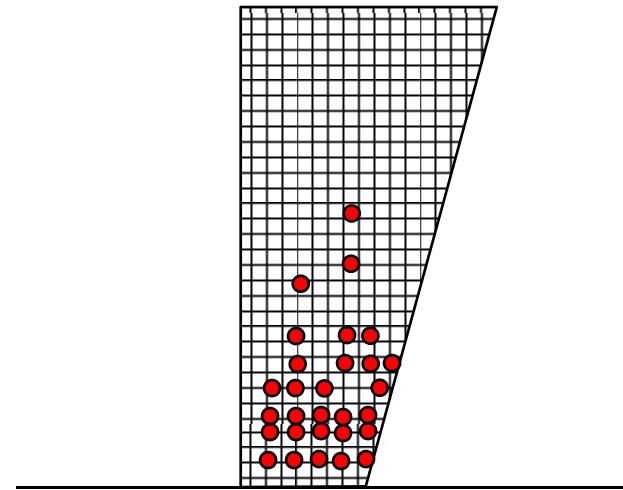
Lecture 9: Fermi-Dirac Statistics

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Carrier Density

Carrier number = Number of states x *filling factor*

↑
Chapters 2-3 Chapter 4



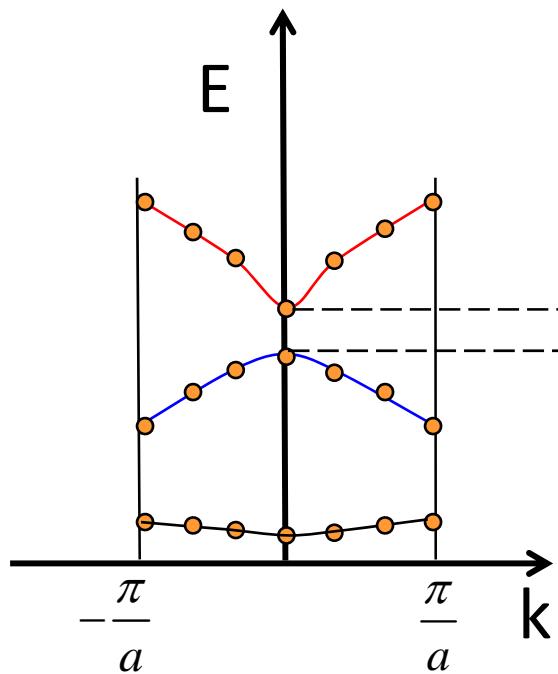
Outline

- 1) Rules of filling electronic states**
- 2) Derivation of Fermi-Dirac Statistics: three techniques
- 3) Intrinsic carrier concentration
- 4) Conclusion

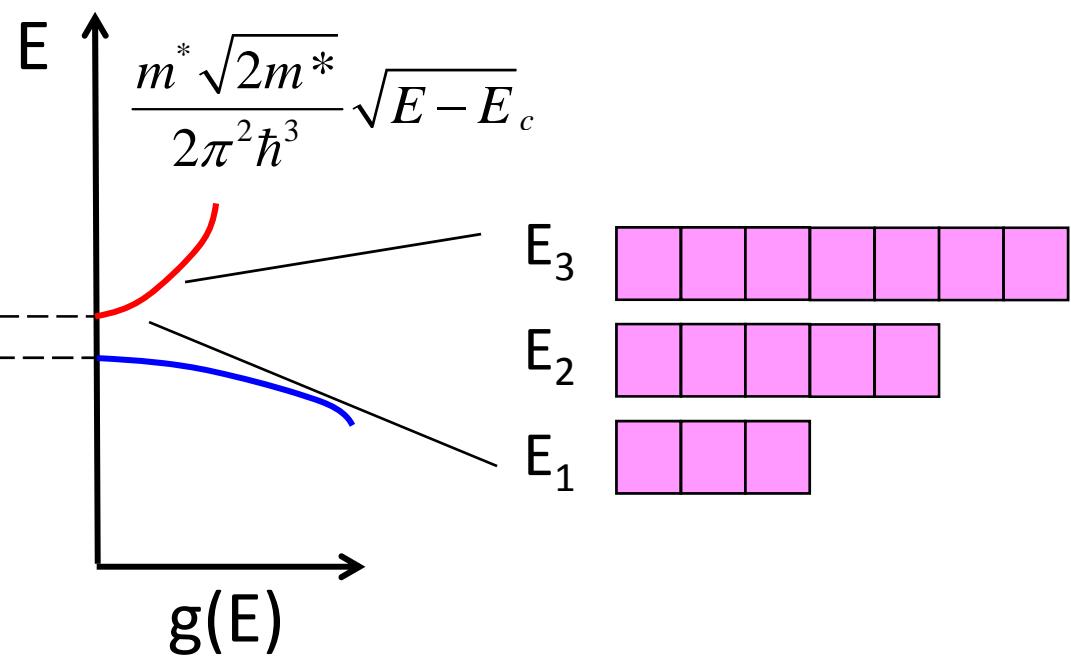
Reference: Vol. 6, Ch. 4 (pages 96-105)

E-k diagram and Electronic States

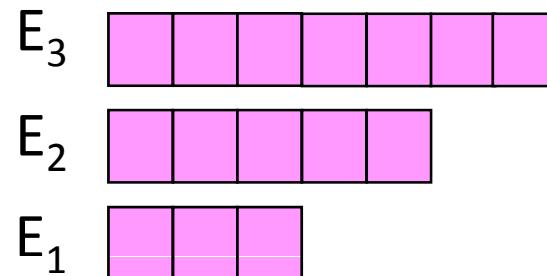
Energy-Band



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 $E_T = \sum_i E_i N_i$

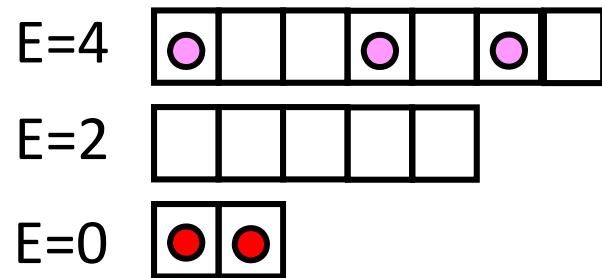
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- 1) Rules of placing electronic states
- 2) Derivation of Fermi-Dirac Statistics: three techniques**
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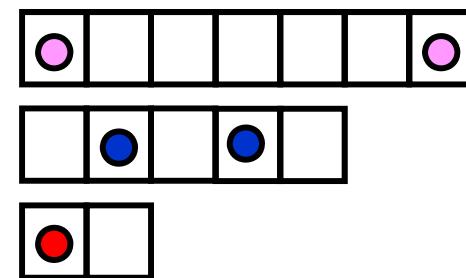
In 1926, Fowler studied collapse of a star to white dwarf by F-D statistics, before Sommerfeld used the F-D statistics to develop a theory of electrons in metals in 1927. Wikipedia has a nice article on this topic.

Illustrative Example: 3 Energy Levels

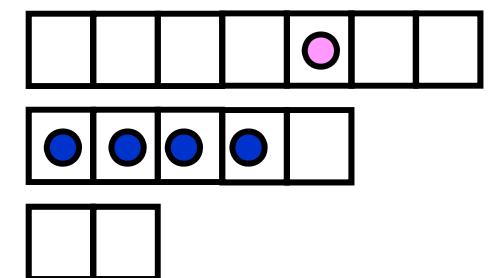
$$N_T = 5 \text{ and } E_T = 12$$



$$N_T = \sum_i N_i$$



$$E_T = \sum_i E_i N_i$$

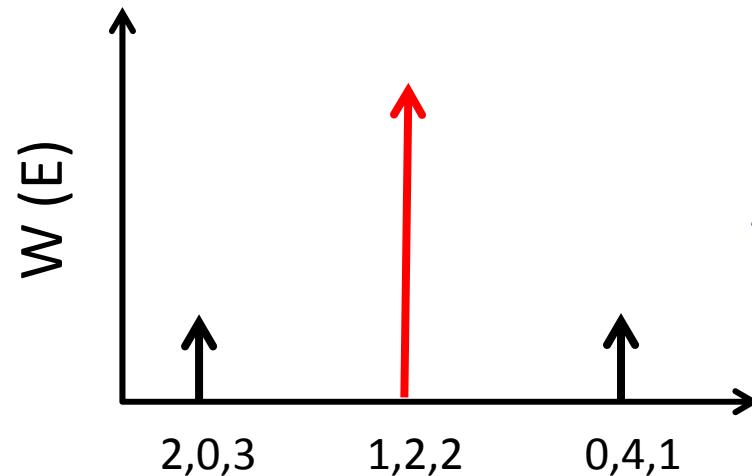
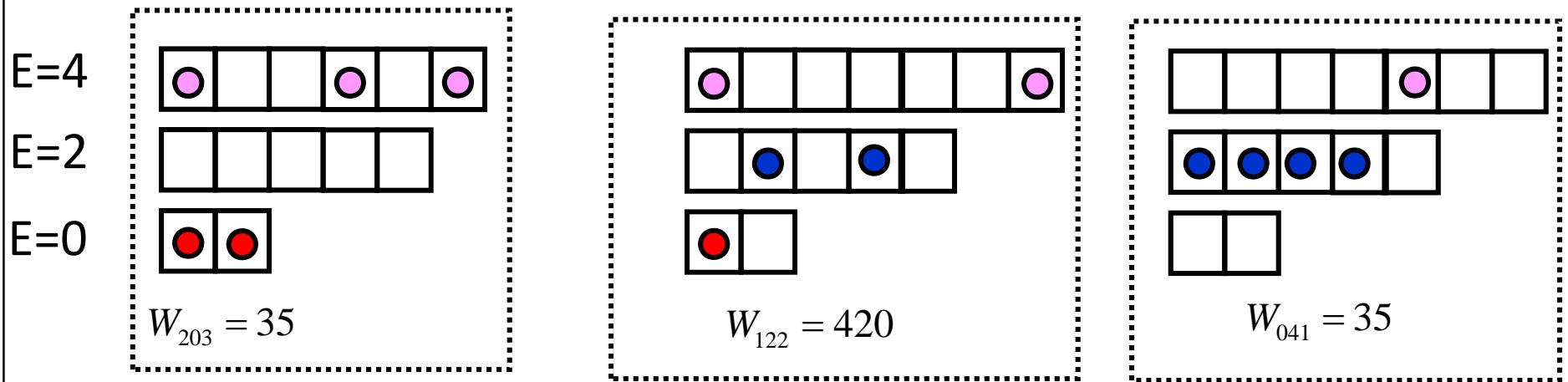


$$W_{203} = \frac{2!}{1!2!} \bullet \frac{5!}{0!5!} \bullet \frac{7!}{3!4!} \\ = 35$$

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

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

Occupation Statistics



*Choose the most
probable configuration.*

Occupation Statistics

$$E=4$$

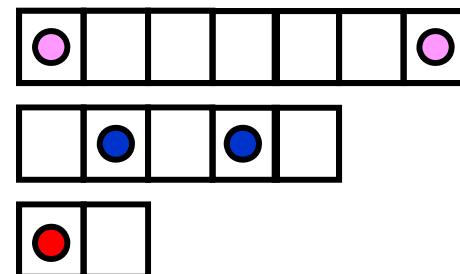
$$f_3^* = \frac{2}{7}$$

$$E=2$$

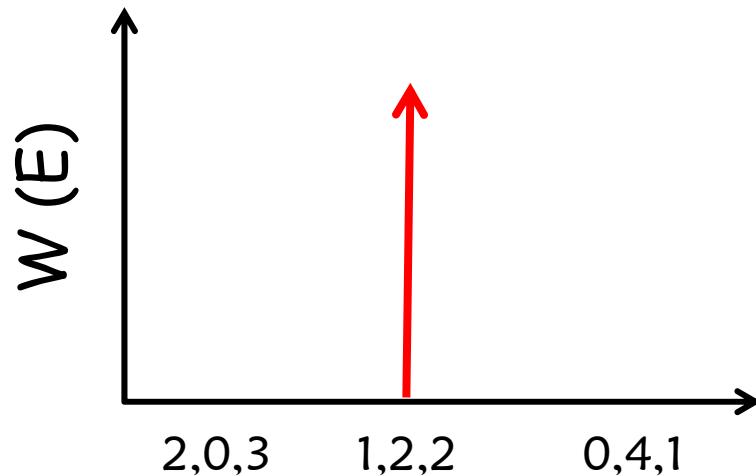
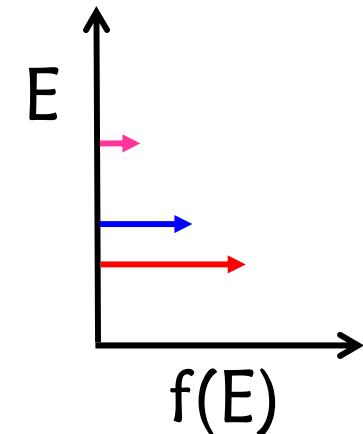
$$f_2^* = \frac{2}{5}$$

$$E=0$$

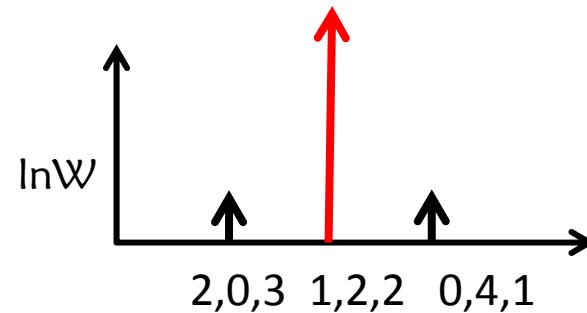
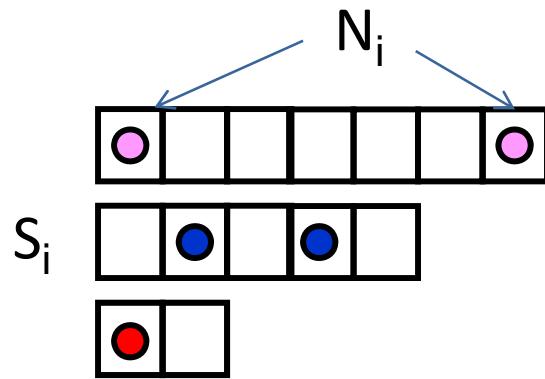
$$f_1^* = \frac{1}{2}$$



$$W_{122} = 420$$



For N-states



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

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

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

Stirling approx.

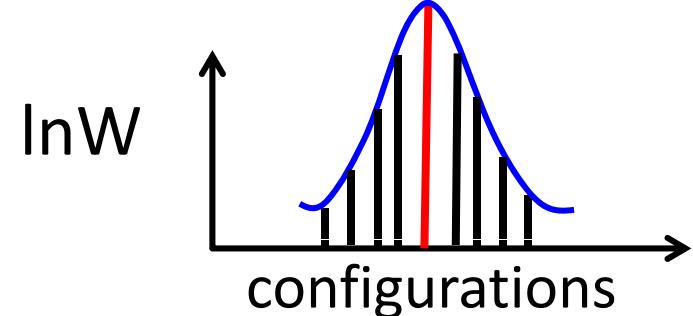
$$\simeq \sum_i [S_i \ln S_i - \textcolor{red}{S}_i - (S_i - N_i) \ln(S_i - N_i) + (\textcolor{red}{S}_i - \textcolor{blue}{N}_i) - N_i \ln N_i + \textcolor{blue}{N}_i]$$

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

Optimization with Lagrange-Multiplier

Choose the most probable configuration.

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



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

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

$$N_T = \sum_i N_i$$

$$E_T = \sum_i E_i N_i$$

Final steps ...

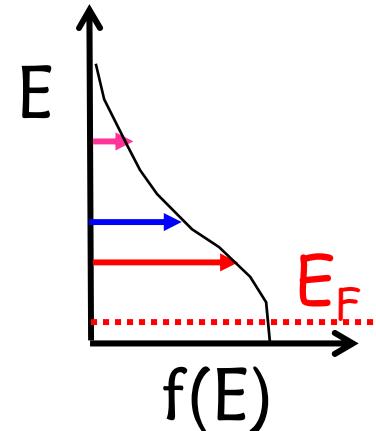
$$\left[\ln\left(\frac{S_i}{N_i} - 1\right) - \alpha - \beta E_i \right] = 0$$

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

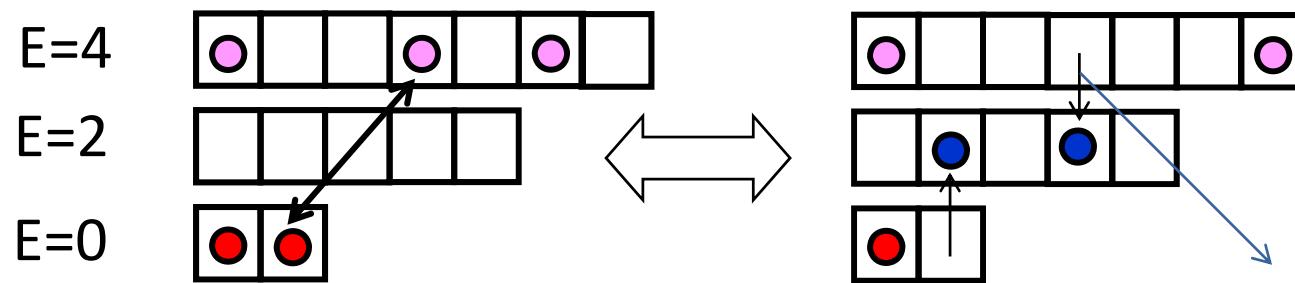
At $E = E_F$, $f(E_F) \equiv \frac{1}{2} \Rightarrow \alpha + \beta E_F = 0$

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

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



Derivation by Detailed Balance

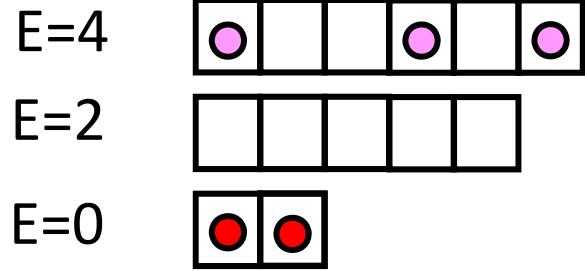


$$A \left\{ f_0(E_1)f_0(E_2)[1 - f_0(E_3)][1 - f_0(E_4)] - f_0(E_3)f_0(E_4)[1 - f_0(E_1)][1 - f_0(E_2)] \right\} = 0$$

$$E_1 + E_2 = E_3 + E_4 \quad \text{Only solution is} \quad f_0(E) = \frac{1}{1 + e^{\beta(E-E_F)}}$$

- Pauli Principle, energy, and number conservation all satisfied

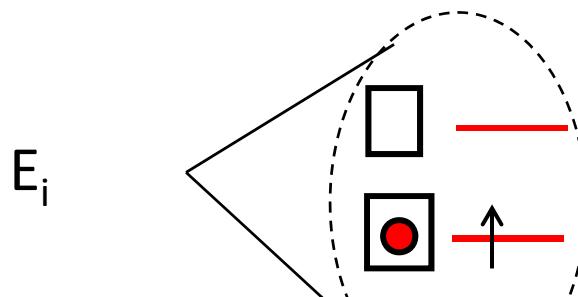
Derivation by Partition Function



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

$$\beta = 1/k_B T$$

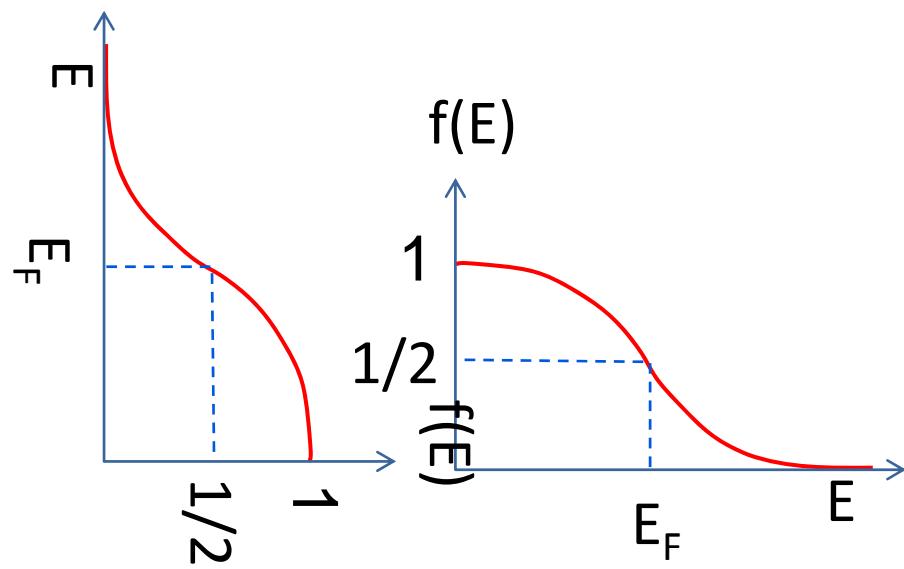
state	E_i	N_i	P_i
	0	0	$e^{-\beta(0 - 0 \times E_F)} / Z$
	1	1	$e^{-\beta(E_i - 1 \times E_F)} / Z$



Derivation by Partition Function

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

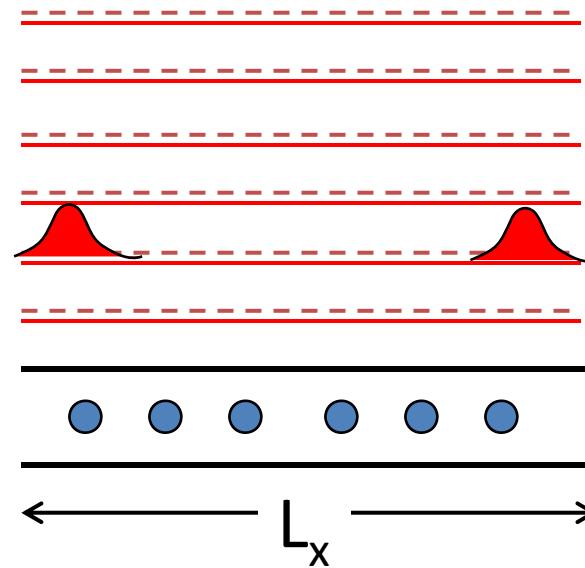
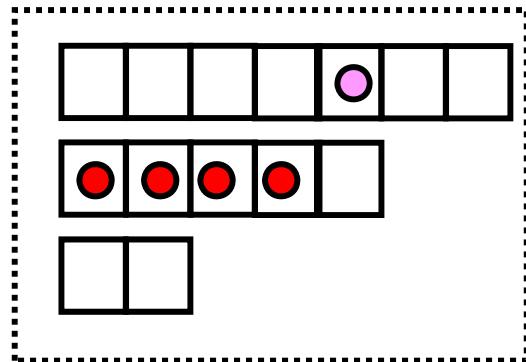
Probability that state is filled



$$\begin{aligned}
 f(E) &= \frac{P_1}{P_0 + P_1} \\
 &= \frac{e^{-(E_i - E_F)/k_B T} / Z}{1/Z + e^{-(E_i - E_F)/k_B T} / Z} \\
 &= \frac{1}{1 + e^{(E_i - E_F)/k_B T}}
 \end{aligned}$$

Few comments on Fermi-Dirac Statistics

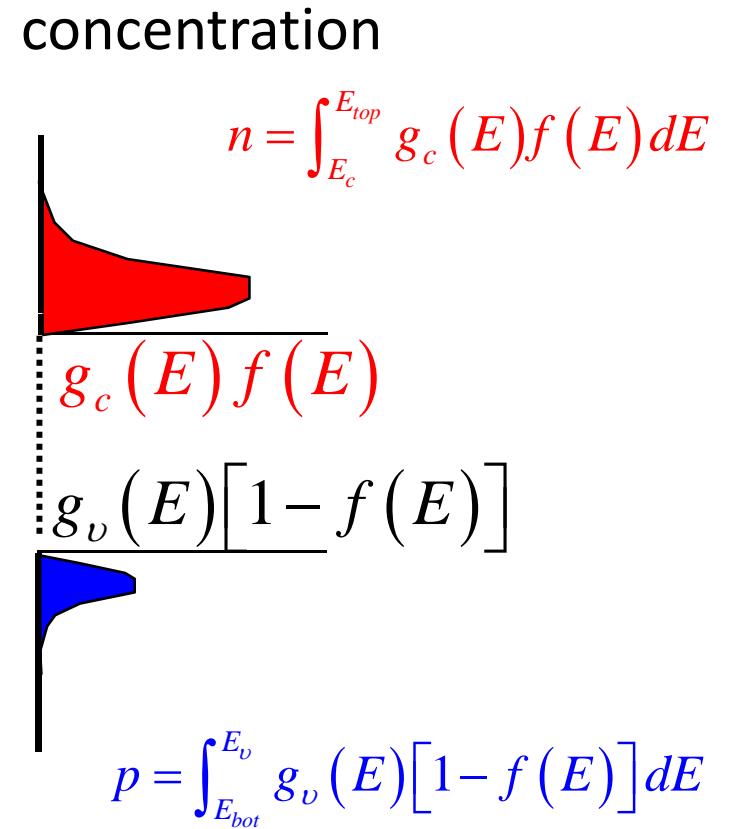
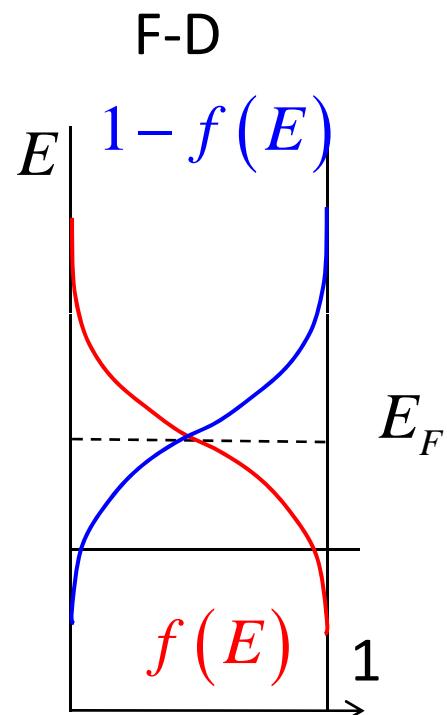
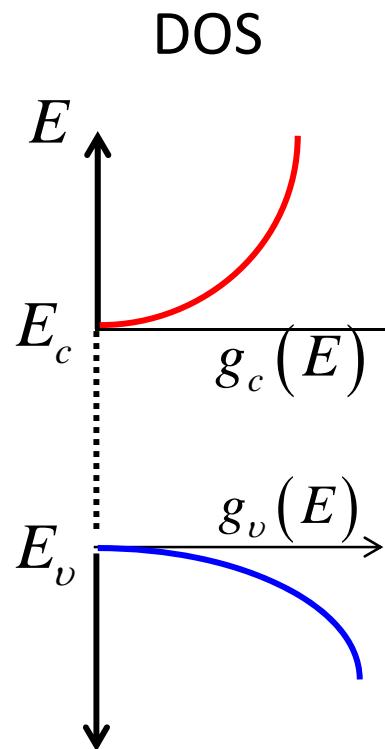
- ❑ Applies to all spin-1/2 particles
- ❑ Information about spin is not explicit; multiply DOS by 2.
May be more complicated for magnetic semiconductors.
- ❑ Coulomb-interaction among particles is neglected,
Therefore it applies to extended solids, not to small molecules



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Carrier Distribution



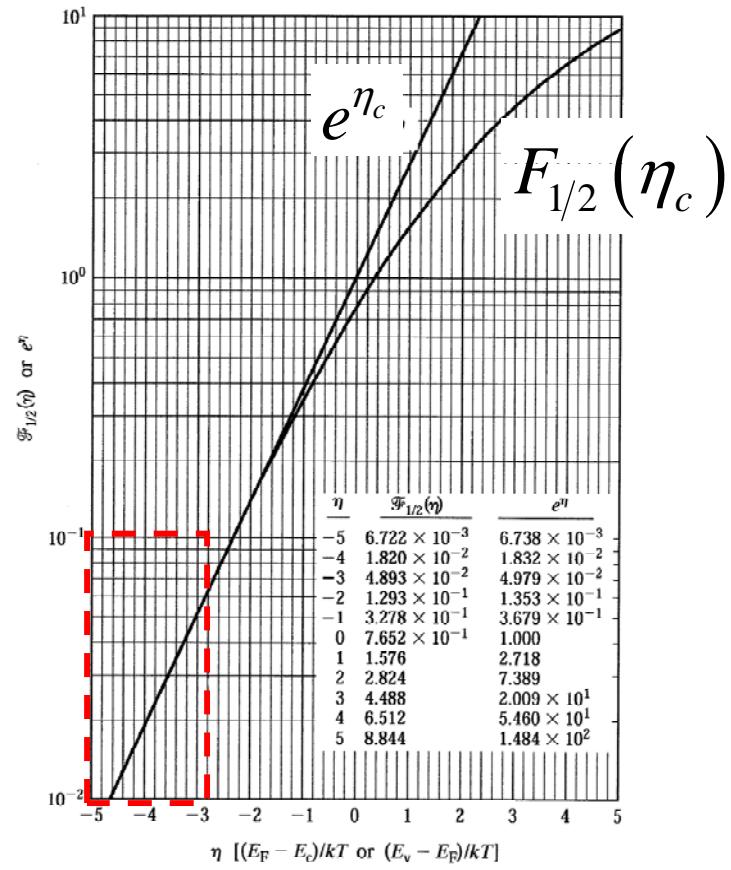
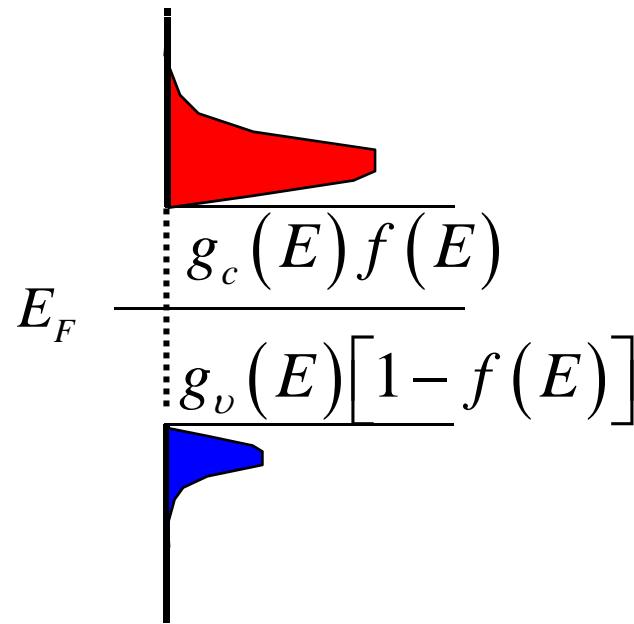
Electron Concentration in 3D solids

$$\begin{aligned}
 n &= \int_{E_c}^{E_{top}} g_c(E) f(E) dE \\
 &= \int_{E_c}^{E_{top}} 2 \times \frac{m_n^* \sqrt{2m_n^*(E - E_C)}}{2\pi^2 \hbar^3} \frac{1}{1 + e^{\beta(E - E_F)}} dE \\
 &\approx \int_{E_c}^{\infty} \frac{m_n^* \sqrt{2m_n^*(E - E_C)}}{\pi^2 \hbar^3} \frac{1}{1 + e^{\beta(E - E_c)} e^{\beta(E_c - E_F)}} dE \\
 &= N_C \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_c) \quad \eta_c \equiv \beta(E_F - E_C)
 \end{aligned}$$

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

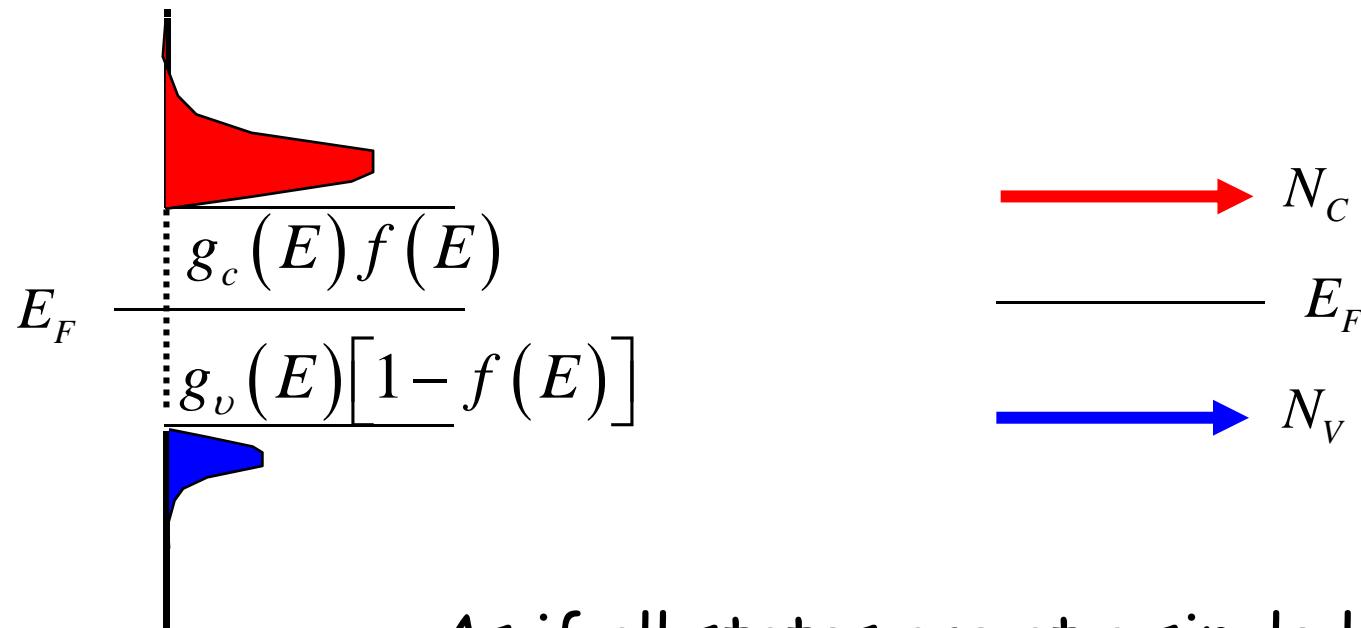
Boltzmann vs. Fermi-Dirac Statistics

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



Effective Density of States

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



As if all states are at a single level E_c

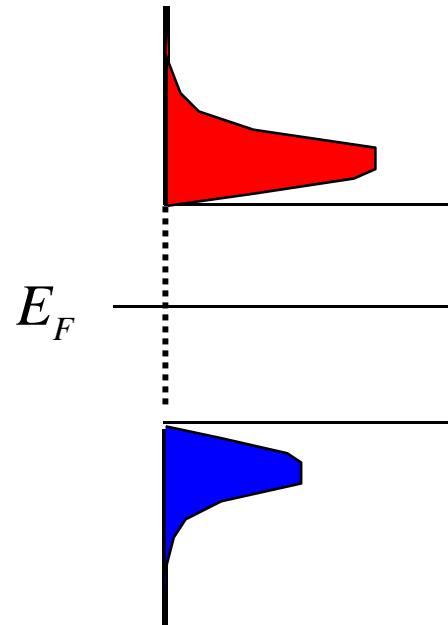
Law of Mass-Action

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

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

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

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



Fermi-Level for Intrinsic Semiconductors

$$n = p = n_i$$

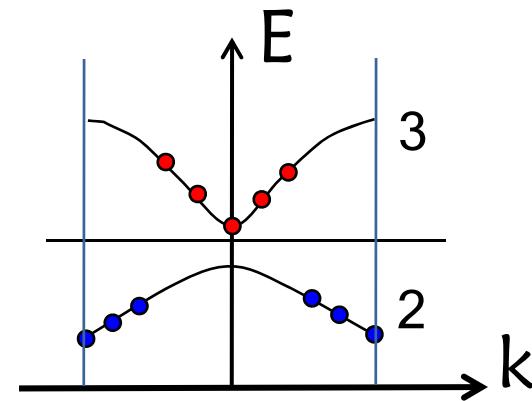
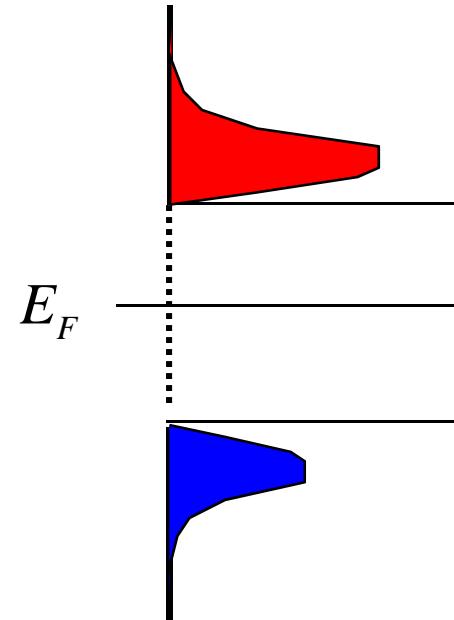
$$n_i^2 = N_C N_V e^{-\beta E_g}$$

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

$$E_F \equiv E_i$$

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

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



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.

We still do not know where E_F is for general semiconductors ...
If we did, we could calculate electron concentration.