Primer on Semiconductors

Unit 3: Equilibrium Carrier Concentrations

Lecture 3.2: Fermi-Dirac integrals

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The Fermi function

The Fermi function gives the probability that a state (if it exists) is occupied in equilibrium.

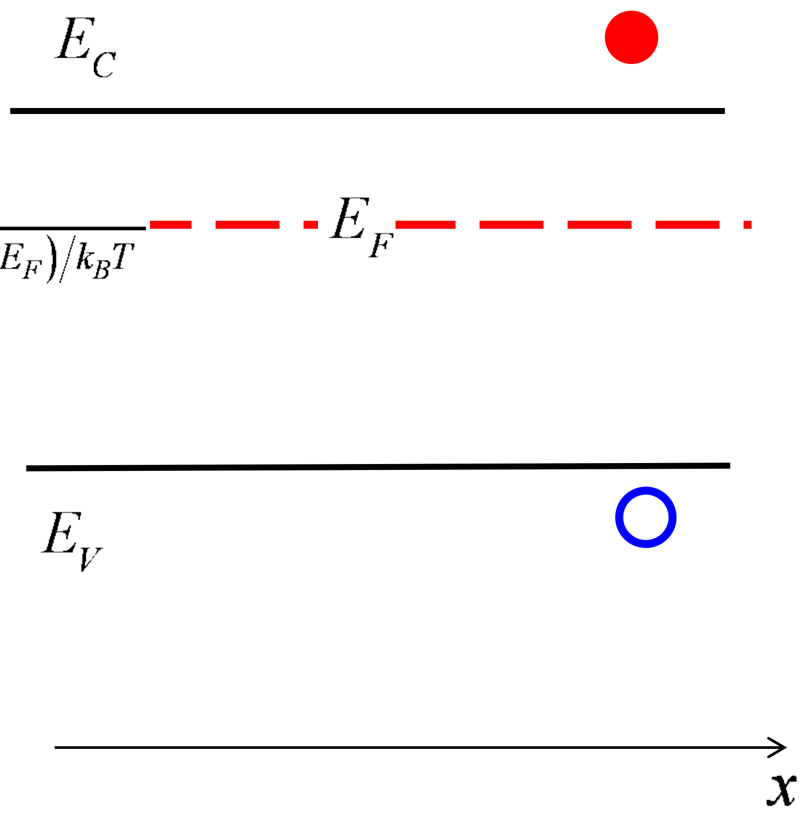
$$\boxed{f_0(E) = \frac{1}{1 + e^{(E - E_F)/k_B T}}}$$

(Fermi function)

The two key parameters in the Fermi function are the Fermi level and the temperature.

Equilibrium carrier densities

$$f_0(E) = \frac{1}{1+e^{(E-E_F)/k_BT}}$$



$$\boxed{n \propto e^{(E_F-E_C)/k_BT}}$$

$$\boxed{p \propto e^{(E_V-E_F)/k_BT}}$$

nondegenerate semiconductor

Two options

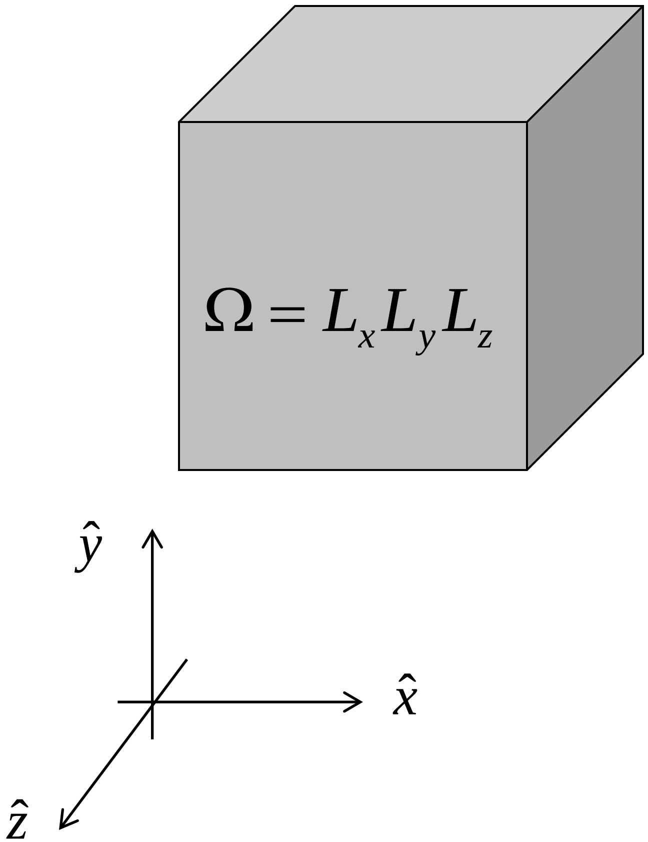
Our goal is to relate the carrier density to the Fermi level and to the properties of the semiconductor.

We can do the calculation two ways:

1) In k-space

2) In energy space

3D bulk semiconductor: k-space



$$N = \sum_{\vec{k}} f_0\left(E_k\right)$$

$$n_0 = \frac{1}{\Omega}\sum_{\vec{k}} f_0\left(E_k\right)$$

$$n_0 = \frac{1}{\Omega}\int_{\vec{k}} f_0\left(E_k\right) N_k d^3k$$

$$N_k = 2\times\left(\frac{\Omega}{8\pi^3}\right) = \frac{\Omega}{4\pi^3}$$

$$\boxed{\sum_{\vec{k}} \bullet \rightarrow \frac{\Omega}{4\pi^3}\int_{BZ} \bullet \, d^3k}$$

Density-of-states in k-space

1D:

$$N_k = 2 \times \left(\frac{L}{2\pi}\right) = \frac{L}{\pi} \qquad dk$$

2D:

$$N_k = 2 \times \left(\frac{A}{4\pi^2}\right) = \frac{A}{2\pi^2} \qquad dk_x dk_y$$

3D:

$$N_k = 2 \times \left(\frac{\Omega}{8\pi^3}\right) = \frac{\Omega}{4\pi^3} \qquad dk_x dk_y dk_z$$

N_k independent of $E(k)$

$$\sum_{\vec{k}} \bullet \rightarrow N_k \int_{BZ} \bullet \, dk$$

(Should include valley degeneracy factor, g_V.)

Energy space (parabolic bands)

$$D_{1D}(E) = g_V \frac{1}{\pi\hbar}\sqrt{\frac{2m^*}{(E-\varepsilon_1)}}\,\Theta(E-\varepsilon_1)$$

$$D_{2D}(E) = g_V \frac{m^*}{\pi\hbar^2}\Theta(E-\varepsilon_1)$$

$$D_{3D}(E) = g_V \frac{m^*\sqrt{2m^*(E-E_C)}}{\pi^2\hbar^3}\Theta(E-E_C)$$

$$\left(E(k) = E_C + \hbar^2 k^2 / 2m^*\right)$$

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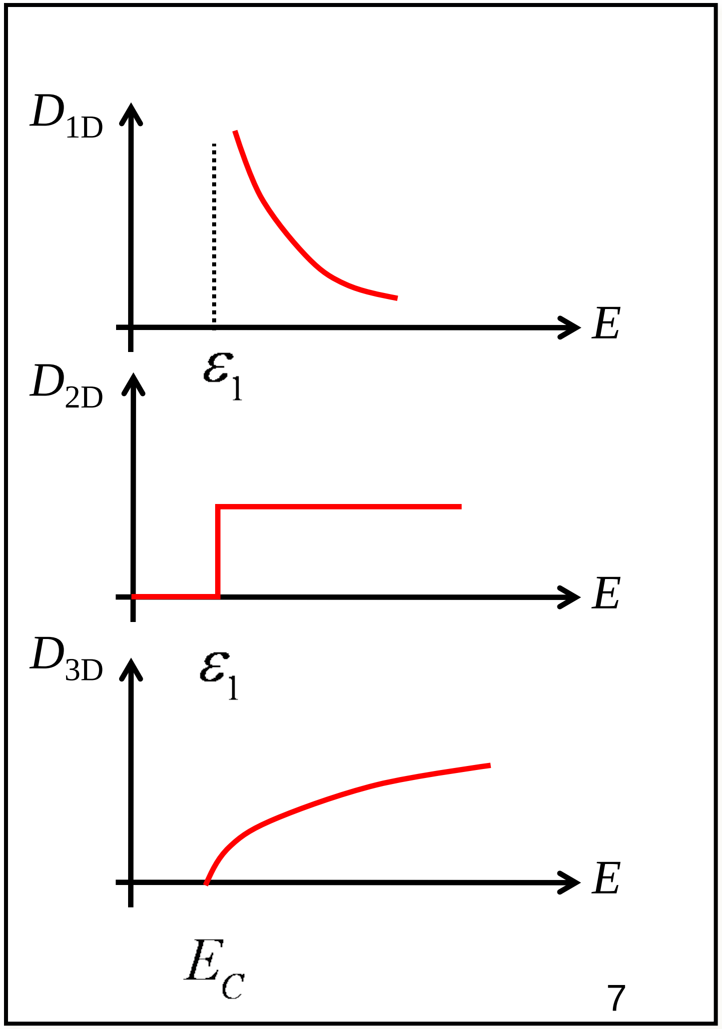
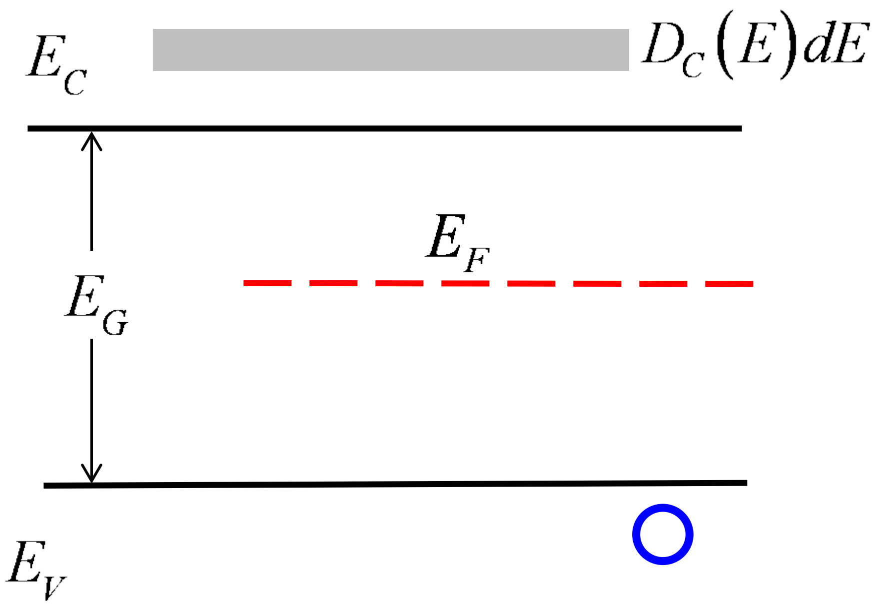


Distribution of electrons in the conduction band



$$n_0(E)dE = f_0(E)D_C(E)dE$$

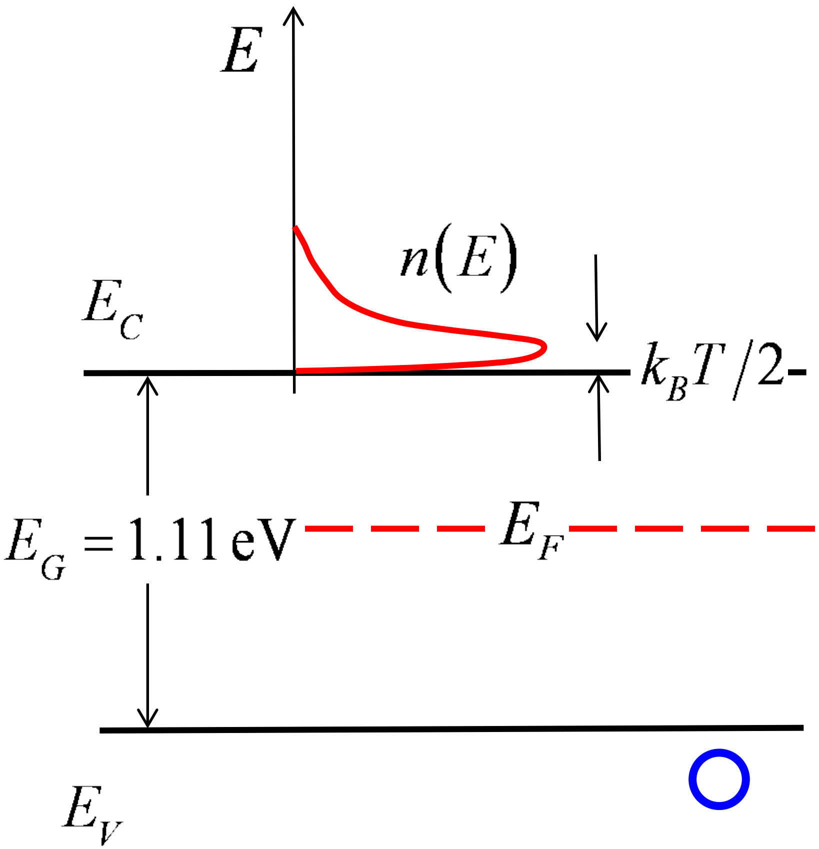
$$f_0(E) = \frac{1}{1+e^{(E-E_F)/k_BT}}$$

$$f_0(E) \approx e^{-(E-E_F)/k_BT}$$

$$D_C(E) \propto \sqrt{E-E_C}$$

$$n_0(E)dE \propto \sqrt{E-E_C}\, e^{-(E-E_F)/k_BT} dE$$

Distribution of electrons in the conduction band



$$n_0(E) \propto \sqrt{E - E_C}\, e^{-(E-E_F)/k_B T}$$

$$\frac{dn_0(E)}{dE} = 0$$

$$E = k_B T/2$$

$$E = 0.013\,\text{eV} \quad T = 300\text{ K}$$

Electrons and holes are very near the band edges.

Compute the electron density

$$n_0 = \int_{E_C}^{\infty} n_0(E)\,dE = \int_{E_C}^{\infty} f_0(E)\,D_C(E)\,dE$$

$$f_0(E) = \frac{1}{1+e^{(E-E_F)/k_BT}}$$

$$D_C(E) = g_V\,\frac{m_n^*\sqrt{2m_n^*(E-E_C)}}{\pi^2\hbar^3}$$

Fermi level and temperature

effective mass and valley degeneracy

Energy space (3D)

$$n_0 = \int_{E_C}^{\infty} f(E) D_C(E)\, dE$$

$$n_0 = \frac{\left(2m^*\right)^{3/2}}{2\pi^2\hbar^3} \int_{E_C}^{\infty} \frac{\left(E - E_C\right)^{1/2}}{1 + e^{\left(E-E_F\right)/k_B T}}\, dE$$

$$n_0 = \frac{\left(2m^* k_B T\right)^{3/2}}{2\pi^2\hbar^3} \int_0^{\infty} \frac{\eta^{1/2}\, d\eta}{1 + e^{\eta - \eta_F}}$$

$$\boxed{n_0 = N_C \mathcal{F}_{1/2}\left(\eta_F\right) \text{cm}^{-3}}$$

$$f_0(E) = \frac{1}{1 + e^{\left(E-E_F\right)/k_B T}}$$

$$D_C(E) = \frac{\left(2m^*\right)^{3/2}}{2\pi^2\hbar^3}\left(E - E_C\right)^{1/2}$$

$$\eta_F = \left(E_F - E_C\right)/k_B T$$

$$\eta = \left(E - E_C\right)/k_B T$$

$$N_C = \frac{1}{4}\left(\frac{2m^* k_B T}{\pi\hbar^2}\right)^{3/2}$$

“effective DOS”

Fermi-Dirac integrals

$$\mathcal{F}_j(\eta_F) \equiv \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\eta^j d\eta}{1+e^{\eta-\eta_F}}$$

$$\Gamma(n) = (n-1)!$$ (*n* integer)

$$\Gamma(1/2) = \sqrt{\pi}$$

$$\Gamma(p+1) = p\Gamma(p)$$

$$\mathcal{F}_j(\eta_F) \to e^{\eta_F} \qquad \eta << 1$$

$$(E_F - E_C)/k_B T << 1$$

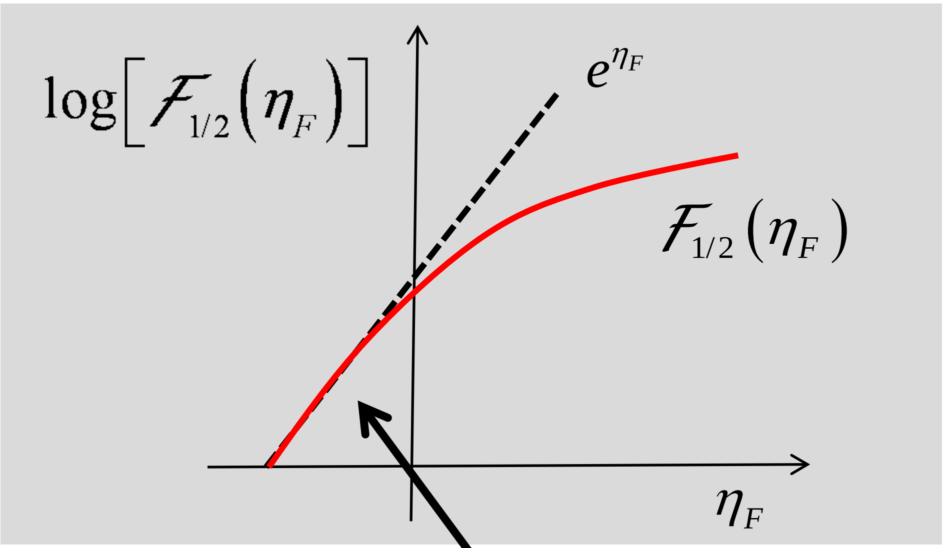
nondegenerate semiconductor

$$\frac{d\mathcal{F}_j}{d\eta_F} = \mathcal{F}_{j-1}$$

don't confuse with…. $F_j(\eta) = \int_0^{+\infty} \frac{x^j dx}{1+e^{x-\eta}}$

For an introduction to Fermi-Dirac integrals, see: "Notes on Fermi-Dirac Integrals," 3rd Ed., by R. Kim and M. Lundstrom) https://www.nanohub.org/resources/5475

Fermi-Dirac integral of order 1/2



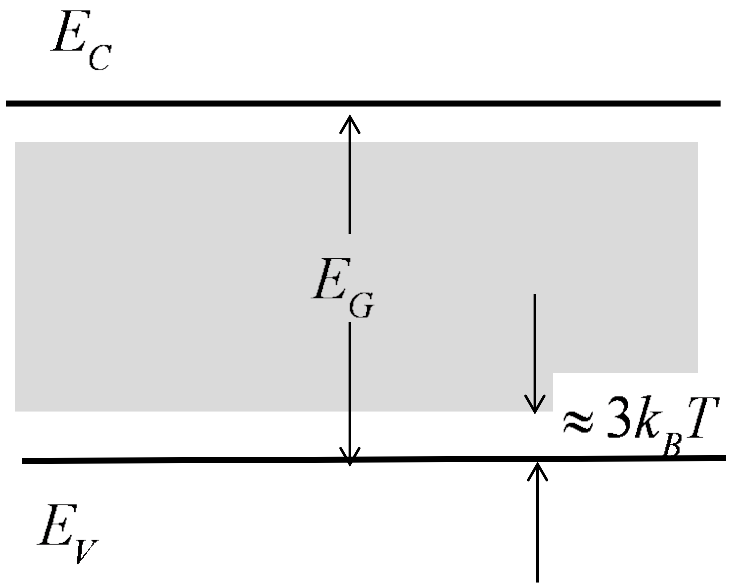
$$\mathcal{F}_{1/2}(\eta_F) \equiv \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\eta^{1/2} d\eta}{1+e^{\eta-\eta_F}}$$

$$\eta_F = (E_F - E_C)/k_B T$$

$$\eta_F << 0 \quad E_F << E_C \quad \mathcal{F}_{1/2}(\eta_F) \rightarrow e^{\eta_F} \quad n_0 = N_C e^{\eta_F} \text{ cm}^{-3}$$

(nondegenerate semiconductor)

Nondegenerate semiconductor



In a nondegenerate semiconductor, the Fermi level is well below the bottom of the conduction band and well above the top of the valence band.

Compute the electron density

$$n_0 = N_C \mathcal{F}_{1/2}(\eta_F)\ \mathrm{cm}^{-3} \qquad \eta_F = (E_F - E_C)/k_B T \qquad N_C = \frac{1}{4}\left(\frac{2m^* k_B T}{\pi\hbar^2}\right)^{3/2}$$

Nondegenerate semiconductors:

$$\eta_F << 0$$

$$E_F << E_C$$

$$\mathcal{F}_{1/2}(\eta_F) \to e^{\eta_F}$$

$$n_0 = N_C e^{\eta_F}\ \mathrm{m}^{-3}$$

Compute the hole density

$$p_0 = \int_{-\infty}^{E_V} \left[1 - f(E)\right] D_V(E)\, dE$$

$$f_0(E) = \frac{1}{1 + e^{(E - E_F)/k_B T}} \qquad D_V(E) = g_V \frac{m_p^* \sqrt{2m_p^*(E_V - E)}}{\pi^2 \hbar^3}$$

$$p_0 = N_V \mathcal{F}_{1/2}(\eta_F)\ \mathrm{m}^{-3} \qquad \eta_F = (E_V - E_F)/k_B T \qquad N_V = \frac{1}{4}\left(\frac{2m_p^* k_B T}{\pi \hbar^2}\right)^{3/2}$$

Nondegenerate semiconductor:

$$\eta_F << 0$$

$$E_F >> E_V$$

$$\mathcal{F}_{1/2}(\eta_F) \to e^{\eta_F} \qquad p_0 = N_V e^{\eta_F}\ \mathrm{m}^{-3}$$

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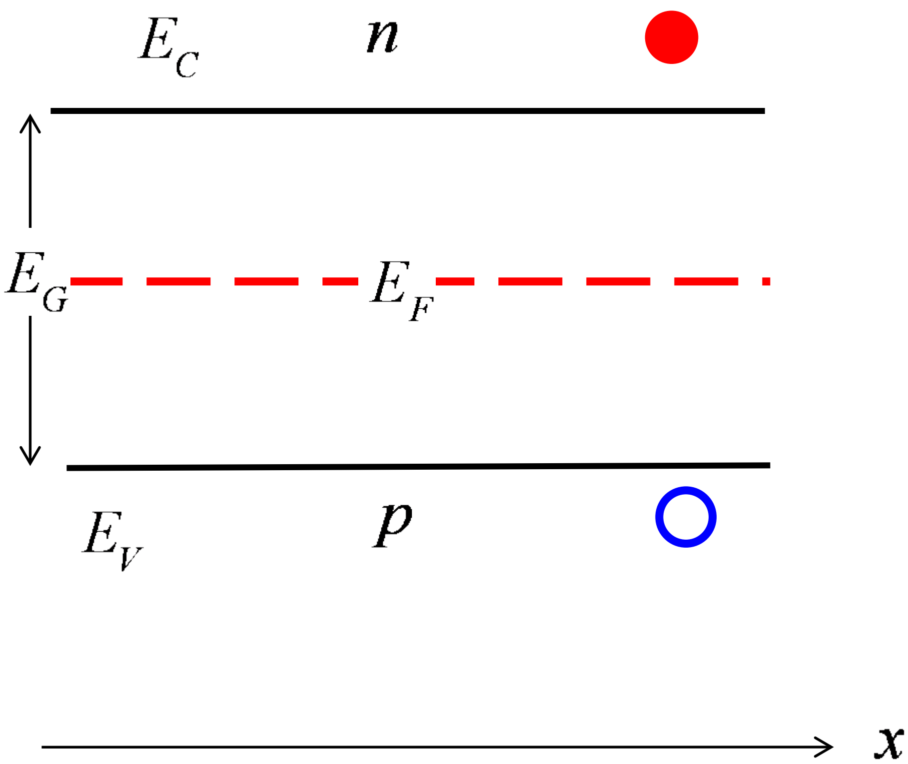
Summary



$$\boxed{n_0 = N_C e^{(E_F - E_C)/k_B T}}$$

$$\boxed{p_0 = N_V e^{(E_V - E_F)/k_B T}}$$

Nondegenerate semiconductor