Notes for
ECE-606: Spring 2013

DOS(E) & Carrier Densities

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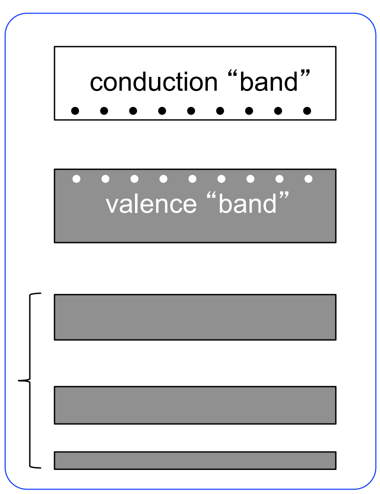
Si energy levels / bands

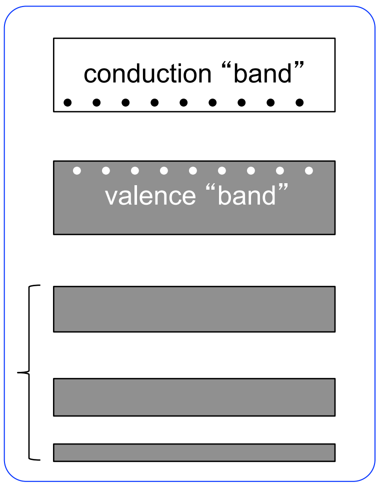


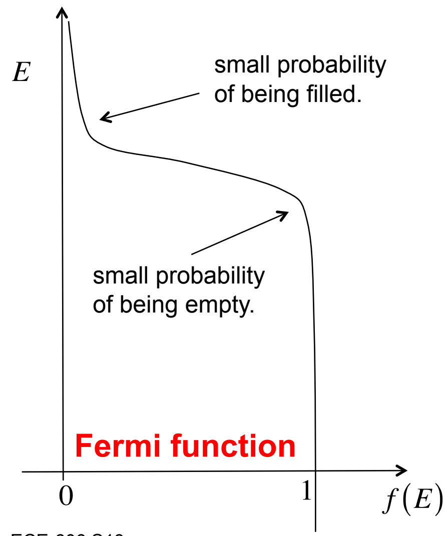
What is the probability, f, that the states in any of these bands are filled?

$4N$ states / band

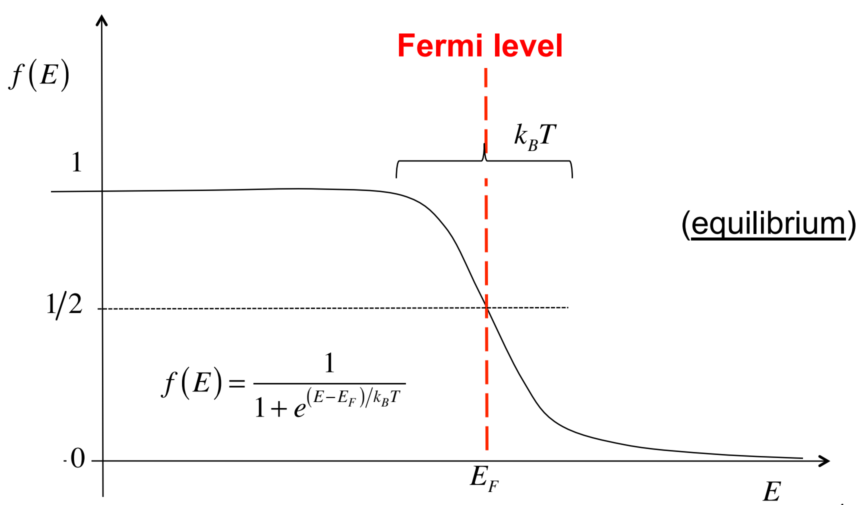
$N = 5 \times 10^{22}$ /cm^3

occupying the bands



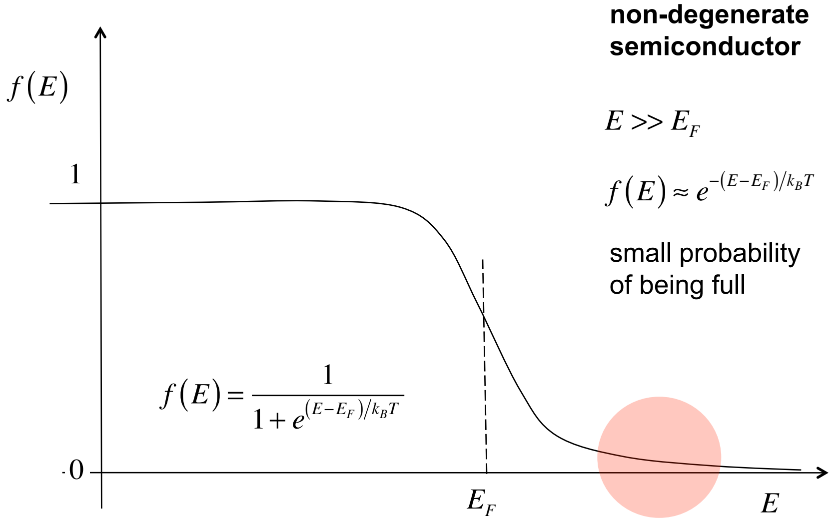


Fermi function



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

conduction band



non-degenerate semiconductor

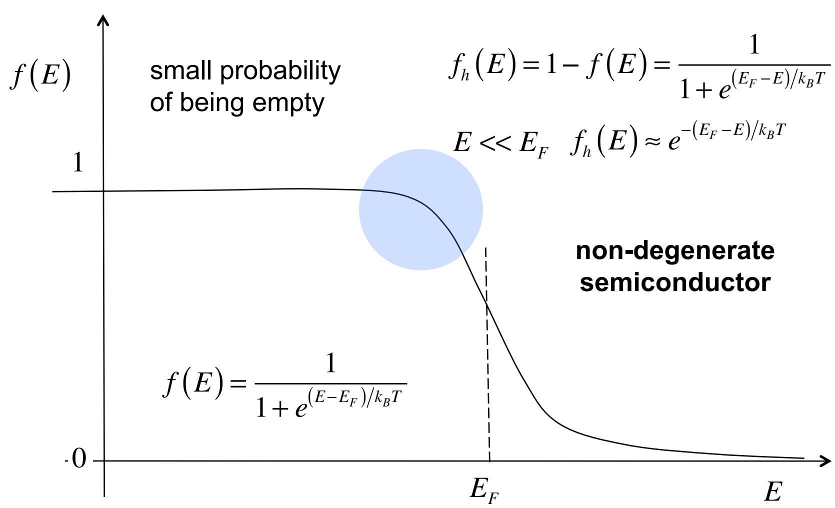
$E >> E_F$

$f(E) \approx e^{-(E-E_F)/k_B T}$

small probability of being full

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

valence band



small probability of being empty

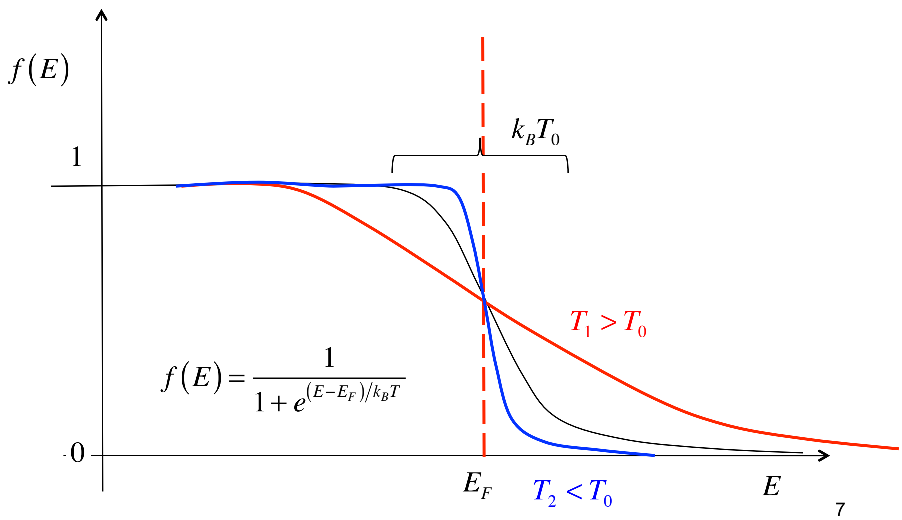
$$f_h(E) = 1 - f(E) = \frac{1}{1+e^{(E_F-E)/k_B T}}$$

$E << E_F \quad f_h(E) \approx e^{-(E_F-E)/k_B T}$

non-degenerate semiconductor

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

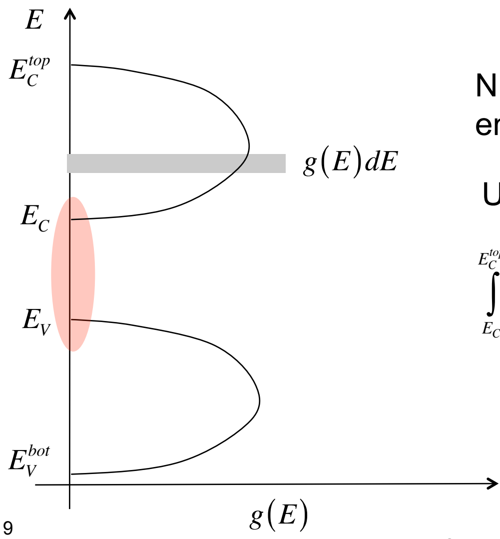
effect of temperature



Fermi function

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

density of states

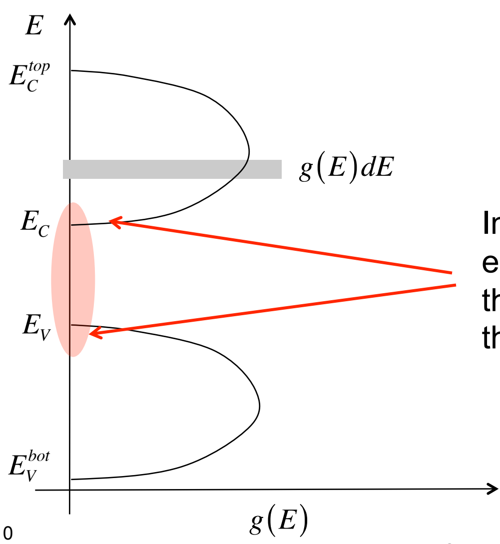


Number of states in an energy range, *dE*

Units: #/J-m^3

$$\int_{E_C}^{E_C^{top}} g(E)dE = 4N$$

density of states near the band edge

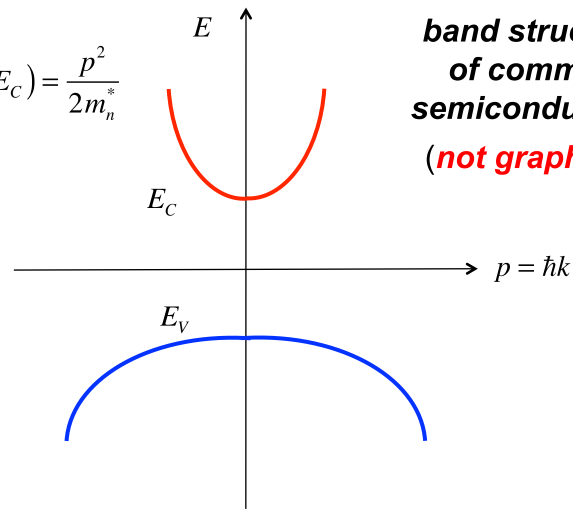


In equilibrium (and near equilibrium), we only need the density of states near the band edge.

Determined by *E*(*k*) near the band edge.

$E(k)$ near the band edges

$$E = \frac{p^2}{2m_0} \rightarrow (E - E_C) = \frac{p^2}{2m_n^*}$$



band structure of common semiconductors

(***not graphene!***)

$$E_V - E = \frac{p^2}{2m_p^*}$$

density of states in k-space

1D:

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

2D:

$$N_k d^2k = 2 \times \frac{A}{(2\pi)^2} d^2k = \frac{A}{2\pi^2} d^2k$$

3D:

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

Things are simple in k-space!

density of states in k-space

$$n_S = \frac{1}{A}\sum_{\vec{k}} f_0\left(E_k\right) \rightarrow \int_{BZ} f_0\left(E_k\right) N_k dk_x dk_y \quad \text{cm}^{-2}$$

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

proportional to area

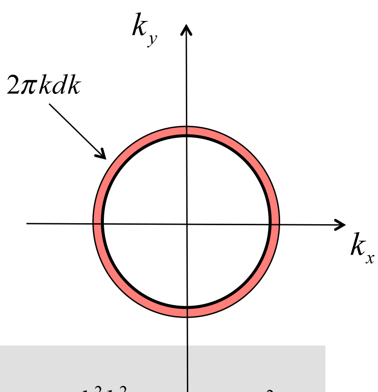
density of states in energy space

$$n_S = \frac{1}{A}\sum_{\vec{k}} f_0\left(E_k\right) \rightarrow \int_{E_{BOT}}^{E_{TOP}} f_0\left(E_k\right) D_{2D}\left(E\right) dE$$

$$\frac{N_k dk}{A} = D_{2D}\left(E\right) dE$$

per unit area

2D DOS(E) – parabolic bands



$$E = \frac{\hbar^2 k^2}{2m^*} \qquad dE = \frac{\hbar^2 k dk}{m^*}$$

$$N_{2D}(k)dk = \left(\frac{A}{(2\pi)^2} \times 2\right) dk_x dk_y$$

$$D_{2D}(E)dE = N_{2D}(k) 2\pi k dk / A$$

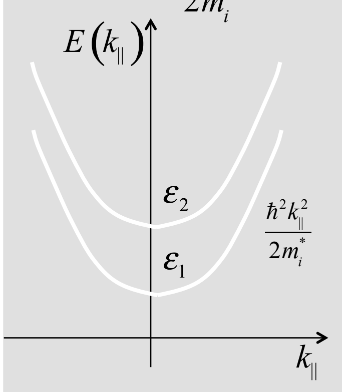
$$D_{2D}(E)dE = \left(\frac{1}{2\pi^2}\right) 2\pi k dk$$

$$D_{2D}(E)dE = \frac{m^*}{\pi\hbar^2} dE$$

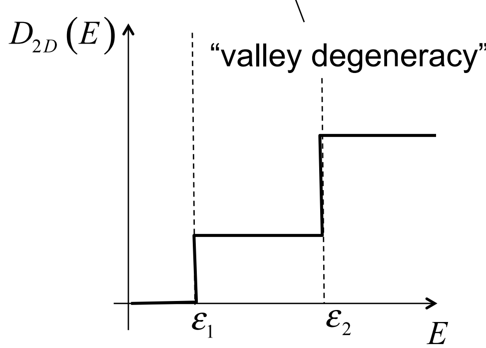
$$\boxed{D_{2D}(E) = \frac{m^*}{\pi\hbar^2}}$$

2D DOS(E) – subbands

$$E = \varepsilon_i + \frac{\hbar^2 k_{\|}^2}{2m_i^*}$$

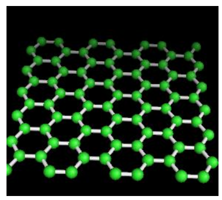


$$D_{2D}^i(E) = g_V \frac{m_i^*}{\pi\hbar^2}$$



2D DOS(E) – graphene

Graphene is a one-atom-thick planar carbon sheet with a honeycomb lattice.

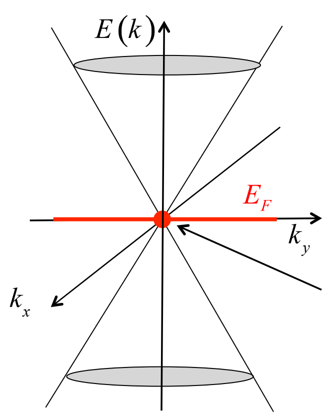


source: CNTBands 2.0 on nanoHUB.org

Graphene has an unusual bandstructure that leads to interesting effects and potentially to useful electronic devices.

graphene: simplified E(k)

We will use a very simple description of the graphene bandstructure, which is a good approximation near the Fermi level.



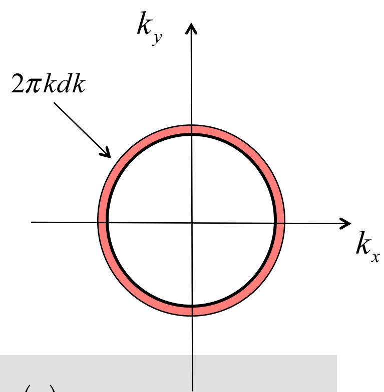
$$E(k) = \pm\hbar\upsilon_F k = \pm\hbar\upsilon_F\sqrt{k_x^2 + k_y^2}$$

$$\upsilon(k) = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \upsilon_F \approx 1\times 10^8 \text{ cm/s}$$

$g_V = 2$ (valley degeneracy)

We will refer to the $E_F > 0$ case, as "n-type graphene" and to the $E_F < 0$ case as "p-type graphene."

2D DOS(E) – graphene



$$E(k) = \hbar\upsilon_F k \qquad dE = \hbar\upsilon_F dk$$

$$k = \frac{E}{\hbar\upsilon_F} \qquad kdk = \frac{EdE}{(\hbar\upsilon_F)^2}$$

$$N_{2D}(k)dk = \left(\frac{A}{(2\pi)^2}\times 2\right)dk_x dk_y$$

$$D_{2D}(E)dE = N_{2D}(k)2\pi kdk/A$$

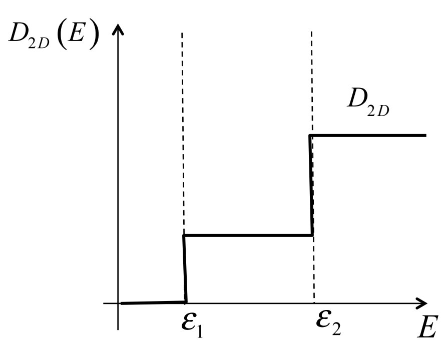
$$D_{2D}(E)dE = \frac{1}{2\pi^2}2\pi kdk$$

$$D_{2D}(E)dE = \frac{E}{\pi(\hbar\upsilon_F)^2}dE$$

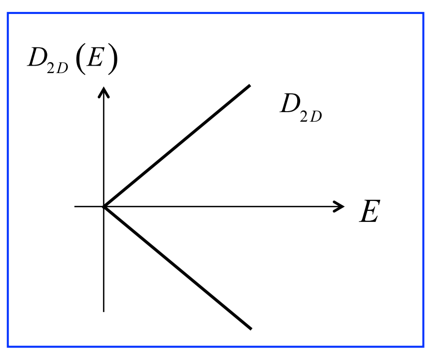
$$D_{2D}(E) = g_V\frac{E}{\pi(\hbar\upsilon_F)^2}$$

2D DOS (E)

parabolic

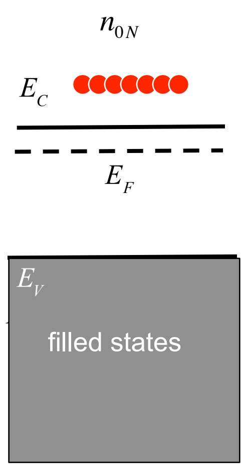


graphene



$$D^i_{2D}(E) = g_V\frac{m_i^*}{\pi\hbar^2} \qquad D_{2D}(E) = g_V\frac{|E|}{\pi\hbar^2\upsilon_F^2} = \frac{2|E|}{\pi\hbar^2\upsilon_F^2}$$

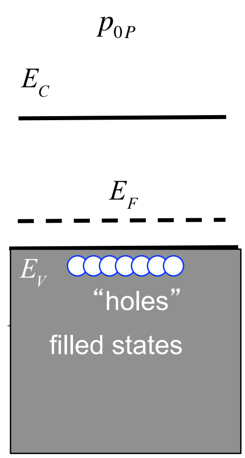
Fermi level (electrochemical potential)



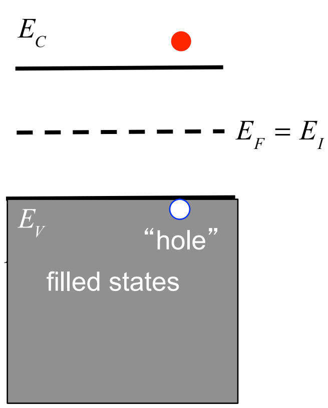
$$f_0(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

$$E << E_F \rightarrow f_0(E) = 1$$

$$E >> E_F \rightarrow f_0(E) = 0$$



intrinsic semiconductor (3D)



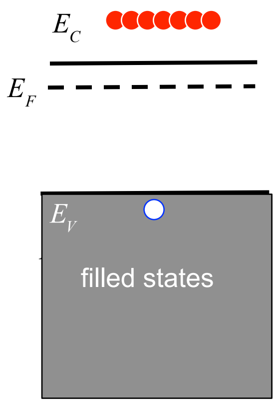
$$n_0 = p_0 = n_i$$

$$n_0 p_0 = n_i^2$$

$$n_i \propto e^{-E_G/k_B T_L}$$

$$n_i(300K) \approx 10^{10} \text{ cm}^{-3}$$

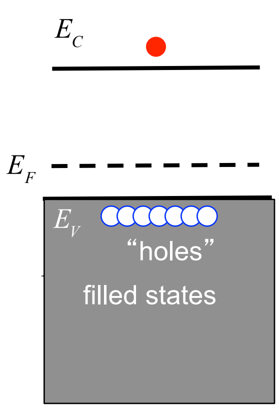
n-type semiconductor (3D)



Expect:

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

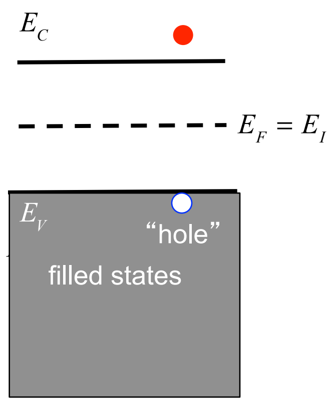
p-type semiconductor (3D)



Expect:

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

intrinsic semiconductor



$$n_0 = p_0 = n_i$$

$$n_0 p_0 = n_i^2$$

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

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

$$n_i^2 = N_C N_V e^{-E_G/k_B T}$$

Example: 2D parabolic energy bands

$$n_S = \int_{E_C}^{E_{TOP}} f_0(E) D_{2D}(E) dE \ \text{cm}^{-2}$$

$$n_S = \int_{E_C}^{E_{TOP}} \frac{1}{1+e^{(E-E_F)/k_B T}} \left(g_V \frac{m_n^*}{\pi \hbar^2} \right) dE \ \text{cm}^{-2}$$

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

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

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

$$D_{2D}(E) = g_V \frac{m_n^*}{\pi \hbar^2}$$

$$\eta \equiv (E - E_C)/k_B T$$

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

Example: 2D parabolic energy bands

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

$$n_S = \left(\frac{g_V m_n^* k_B T}{\pi\hbar^2} \right) \int_0^{\infty} \frac{d\eta}{1 + e^{\eta - \eta_F}}$$

$$\int_0^{\infty} \frac{d\eta}{1 + e^{\eta - \eta_F}} = \ln\left(1 + e^{\eta_F}\right) = \mathcal{F}_0\left(\eta_F\right)$$

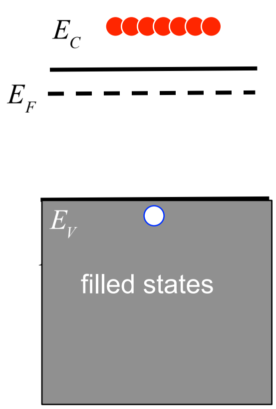
$$n_S = \left(\frac{g_V m_n^* k_B T}{\pi\hbar^2} \right) \mathcal{F}_0\left(\eta_F\right) = N_C^{2D}\ \mathcal{F}_0\left(\eta_F\right)$$

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

$$dE = k_B T d\eta$$

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

N-type semiconductor (2D parabolic)



$$n_S = N_C^{2D}\ \mathcal{F}_0\left(\eta_F\right)$$

$$N_C^{2D} = \left(\frac{g_V m_n^* k_B T}{\pi\hbar^2} \right)$$

$$\mathcal{F}_0\left(\eta_F\right) = \ln\left(1 + e^{\eta_F}\right)$$

$\eta_F << 0 \quad E_F << E_C :$

$\mathcal{F}_0\left(\eta_F\right) \rightarrow e^{\eta_F}$

$n_S = N_C^{2D}\ e^{\eta_F}$ non-degenerate semiconductor

Example: 2D linear energy bands

$$n_S = \int_0^{E_{TOP}} f_0(E) D_{2D}(E) dE \ \ \text{cm}^{-2}$$

$$n_S = \int_{E_C}^{E_{TOP}} \frac{1}{1+e^{(E-E_F)/k_BT}} \left(\frac{2E}{\pi\hbar^2\upsilon_F^2} \right) dE \ \ \text{cm}^{-2}$$

$$n_S = \left(\frac{2}{\pi\hbar^2\upsilon_F^2} \right) \int_0^\infty \frac{EdE}{1+e^{(E-E_F)/k_BT}}$$

$$n_S = \left(\frac{2}{\pi\hbar^2\upsilon_F^2} \right) \int_0^\infty \frac{k_BT\eta(k_BTd\eta)}{1+e^{\eta-\eta_F}}$$

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

$$D_{2D}(E) = \frac{2E}{\pi\hbar^2\upsilon_F^2}$$

$$\eta \equiv E/k_BT$$

$$\eta_F \equiv E_F/k_BT$$

Example: 2D linear energy bands

$$n_S = \frac{2}{\pi}\left(\frac{k_BT}{\hbar\upsilon_F} \right)^2 \int_0^\infty \frac{\eta d\eta}{1+e^{\eta-\eta_F}}$$

$$\mathcal{F}_1(\eta_F) \equiv \int_0^\infty \frac{\eta d\eta}{1+e^{\eta-\eta_F}}$$

$$n_S = N_C^{graphene} \mathcal{F}_1(\eta_F) \ \text{cm}^{-2}$$

$$N_C^{graphene} = \frac{2}{\pi}\left(\frac{k_BT}{\hbar\upsilon_F} \right)^2$$

$$\eta \equiv E/k_BT$$

$$\eta_F \equiv E_F/k_BT$$

Fermi-Dirac integrals

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

$$\Gamma(n) = (n-1)! \qquad (n \text{ integer})$$

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

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

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

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

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

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

exercises

$$u = \frac{\langle E - E_C \rangle}{n_S} = \frac{\int_{E_C}^{\infty} (E - E_C) f_0(E) D_{2D}(E) dE}{\int_{E_C}^{\infty} f_0(E) D_{2D}(E) dE} \text{ J}$$

1) T = 0 K
2) Under non-degenerate conditions
3) In general