Si energy levels / bands

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

- conduction “band”
- valence “band”

4\(N\) states / band

\[ N = 5 \times 10^{22} / \text{cm}^3 \]
occupying the bands

conduction “band”

valence “band”

small probability of being filled.

small probability of being empty.

Fermi function

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

Fermi level

\[ E_F \]

(equilibrium)
conduction band

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

small probability of being full

\[ f(E) = e^{-(E - E_F) / k_B T} \]

non-degenerate semiconductor

valence band

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

small probability of being empty

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

non-degenerate semiconductor

\[ f_h(E) = e^{-(E - E_F) / k_B T} \]
effect of temperature

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

Fermi function

\[ f(E) = \frac{1}{1 + e^{(E - E_F)/k_B T}} \]
Number of states in an energy range, \( dE \)

Units: \( \#/\text{J-m}^3 \)

\[
\int_{E_c}^{E^{\text{top}}} g(E) dE = 4N
\]

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

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

$E_C$

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

$p = \hbar k$

**band structure of common semiconductors**
**not graphene!**

Density of states in k-space

1D:

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

2D:

$$N_x d^2 k = 2 \times \left( \frac{A}{(2\pi)^2} \right) d^2 k = \frac{A}{2\pi^2} d^2 k$$

3D:

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

Things are simple in k-space!
density of states in k-space

\[ n_S = \frac{1}{A} \sum_k f_0(E_k) \to \int_{BZ} f_0(E_k) N_k dk_x dk_y \text{ cm}^{-2} \]

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

proportional to area

density of states in energy space

\[ n_S = \frac{1}{A} \sum_k f_0(E_k) \to \int_{E_{TOP}}^{E_{BOT}} f_0(E_k) D_{2D}(E) dE \]

\[ \frac{N_k dk}{A} = D_{2D}(E) dE \]

per unit area
2D DOS(E) – parabolic bands

\[ E = \frac{\hbar^2 k^2}{2m} \]

\[ dE = \frac{\hbar^2 k dk}{m} \]

\[ N_{2D}(k) dk = \left( \frac{A}{(2\pi)^2} \right) \times 2 \, dk, \, dk_y \]

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

\[ D_{2D}(E)dE = \left( \frac{1}{2\pi^2} \right) 2\pi kdk \]

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

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

2D DOS(E) – subbands

\[ E = \varepsilon_i + \frac{\hbar^2 k_{i}^2}{2m_i} \]

\[ E(k_x) \]

\[ \varepsilon_1 \]

\[ \varepsilon_2 \]

\[ \hbar^2 k_{i}^2 \]

\[ 2m_i \]

\[ D_{2D}(E) \]

\[ V \]

\[ D_{2D}^V(E) = g_v \frac{m^*_v}{\pi\hbar^2} \]

“valley degeneracy”
Graphene is a one-atom-thick planar carbon sheet with a honeycomb lattice. Graphene has an unusual bandstructure that leads to interesting effects and potentially to useful electronic devices.

source: CNTBands 2.0 on nanoHUB.org

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

\[ N_{2D}(k)dk = \frac{A}{(2\pi)^2} \times 2 \, dk_x, \]

\[ D_{2D}(E)dE = N_{2D}(k)2\pi kdE/A \]

\[ D_{2D}(E)dE = \frac{1}{2\pi^2} 2\pi kdE \]

\[ D_{2D}(E) = g_V \frac{E}{\pi(hv_F)^2} \]

Lundstrom ECE-606 S13

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2D DOS (E)

parabolic

\[ D_{2D}^p(E) = g_V \frac{m^*}{\pi\hbar^2} \]

graphene

\[ D_{2D}^g(E) = g_V \frac{|E|}{\pi\hbar^2v_F^2} = \frac{2|E|}{\pi\hbar^2v_F^2} \]

Lundstrom ECE-606 S13
Fermi level (electrochemical potential)

\[ n_{0N} \]

\[ E_C \]

\[ E_F \]

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

\[ E << E_F \rightarrow f_0(E) = 1 \]

\[ E >> E_F \rightarrow f_0(E) = 0 \]

\[ p_{0P} \]

\[ E_C \]

\[ E_F \]

intrinsic semiconductor (3D)

\[ E_C \]

\[ E_F = E_I \]

\[ n_0 = p_0 = n_i \]

\[ n_0 p_0 = n_i^2 \]

\[ n_i \propto e^{-E_i/k_B T} \]

\[ n_i (300 \, K) \approx 10^{10} \, \text{cm}^{-3} \]
n-type semiconductor (3D)

Expect:

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

p-type semiconductor (3D)

Expect:

\[ p_0 = N_V e^{(E_F - E_V)/k_B T} \]
intrinsic semiconductor

\[ E_C \]

\[ E_F = E_i \]

\[ n_0 = p_0 = n_i \]

\[ n_0 p_0 = n_i^2 \]

\[ n_0 = N_c e^{(E_F - E_C)/k_B T} \]

\[ p_0 = N_v e^{(E_F - E_V)/k_B T} \]

\[ n_i^2 = N_c N_v e^{-E_i/k_B T} \]

Example: 2D parabolic energy bands

\[ n_S = \int_{E_C}^{E_F} f_0(E) D_{2D}(E) dE \text{ cm}^{-2} \]

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

\[ D_{2D}(E) = g_v \frac{m_n^*}{\pi \hbar^2} \]

\[ \eta \equiv \frac{E - E_C}{k_B T} \]

\[ \eta_F \equiv \frac{(E_F - E_C)}{k_B T} \]
Example: 2D parabolic energy bands

\[ n_s = \left( g_v \frac{m^*_n}{\pi \hbar^2} \right) \int_{E_C}^{\infty} \frac{dE}{1 + e^{(E-E_C+E_F)/k_B T}} \]

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

\[ dE = k_B T d\eta \]

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

\[ n_s = \left( g_v m^*_n k_B T \right) \int_0^\infty \frac{d\eta}{1 + e^{\eta - \eta_F}} \]

\[ \int_0^\infty \frac{d\eta}{1 + e^{\eta - \eta_F}} = \ln\left(1 + e^{\eta_F}\right) = F_0(\eta_F) \]

\[ n_s = \left( g_v m^*_n k_B T \right) F_0(\eta_F) = N_c^{2D} F_0(\eta_F) \]

N-type semiconductor (2D parabolic)

\[ n_s = N_c^{2D} F_0(\eta_F) \]

\[ N_c^{2D} = \left( g_v m^*_n k_B T \right) \frac{1}{\pi \hbar^2} \]

\[ F_0(\eta_F) = \ln\left(1 + e^{\eta_F}\right) \]

\[ \eta_F \ll 0 \quad E_F \ll E_C; \quad F_0(\eta_F) \rightarrow e^{\eta_F} \]

\[ n_s = N_c^{2D} e^{\eta_F} \quad \text{non-degenerate semiconductor} \]
Example: 2D linear energy bands

\[ n_S = \int_0^{E_{top}} f_0(E) D_{2D}(E) dE \text{ cm}^{-2} \]

\[ n_S = \int_{E_c}^{E_{top}} \frac{1}{1 + e^{(E-E_F)/k_B T}} \left( \frac{2E}{\pi \hbar^2 v_F^2} \right) dE \text{ cm}^{-2} \]

\[ n_S = \left( \frac{2}{\pi \hbar^2 v_F^2} \right) \int_0^\infty \frac{E dE}{1 + e^{(E-E_F)/k_B T}} \]

\[ n_S = \left( \frac{2}{\pi \hbar^2 v_F^2} \right) \int_0^\infty \frac{k_B T \eta (k_B T d\eta)}{1 + e^{\eta - \eta_F}} \]

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

\[ D_{2D}(E) = \frac{2E}{\pi \hbar^2 v_F^2} \]

\[ \eta = E/k_B T \]

\[ \eta_F = E_F/k_B T \]

\[ n_S = N_{\text{graphene}} \mathcal{F}_1(\eta_F) \text{ cm}^{-2} \]

\[ N_{\text{graphene}} = \frac{2}{\pi} \left( \frac{k_B T}{\hbar v_F} \right)^2 \]

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

\[ n_S = N_{\text{graphene}} \mathcal{F}_1(\eta_F) \text{ cm}^{-2} \]
Fermi-Dirac integrals

\[ F_j(\eta_F) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\eta^j d\eta}{1 + e^{\eta - \eta_F}} \]

\[ \Gamma(n) = (n-1)! \quad (n \text{ integer}) \]

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

\[ \Gamma(p+1) = p\Gamma(p) \]

\[ F_j(\eta_F) \rightarrow e^{\eta_F} \quad \eta << 1 \]

\[ \frac{dF_j}{d\eta_F} = F_{j-1} \]

Don’t confuse with….

\[ F_j(\eta) = \int_0^\infty \frac{x^j dx}{1 + e^{x - \eta}} \]


exercises

\[ u = \left\langle E - E_C \right\rangle \]

\[ n_s = \frac{\int_{E_C}^\infty (E - E_C) f_0(E) D_{2D}(E) dE}{\int_{E_C}^\infty f_0(E) D_{2D}(E) dE} \]

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