1) Assume $T = 0$K and work out the electron density per unit area for two cases:

i) A 2D semiconductor with parabolic energy bands and an effective mass of $m^*$. (Assume a valley degeneracy of 2.)

ii) Graphene, where we consider $E > 0$ to be the conduction band. ($E = 0$ is where the bands cross, the so-called Dirac point.)

1a) Express your two answers in terms of the Fermi energy, and show that they are different.

1b) Express your two answers in terms of the Fermi wavevector and show that they are the same.

Solution:

1a) In terms of energy:

Case i): parabolic energy bands: DOS:

$$D_{2D}(E) = g_V \frac{m^*}{\pi h^*} = \frac{2m^*}{\pi h^*} \left( E > E_c = 0 \right)$$

$$n_s = \int_{E_c}^{\infty} D_{2D}(E)f_0(E) dE = n_s = \int_0^{E_F} D_{2D}(E) dE \quad (T = 0 \text{ K})$$

$$n_s = \int_0^{E_F} g_V \frac{m^*}{\pi h^*} dE = \frac{2m^*}{\pi h^*} E_F$$

$$n_s = g_V \frac{m^*}{\pi h^*} E_F = \frac{2m^*}{\pi h^*} E_F$$

Case ii): graphene: DOS:

$$D_{2D}(E) = g_V \frac{E}{\pi h^2 v_F^2} = \frac{2E}{\pi h^2 v_F^2} \left( E > 0 \right) \quad \text{(valley degeneracy is 2 for graphene)}$$

Aside: Note that if we define the effective mass of graphene by $E \equiv m^* v_F^2$, then we could use the parabolic band DOS and get the right DOS for graphene!

$$n_s = \int_{E_c}^{\infty} D_{2D}(E)f_0(E) dE = n_s = \int_0^{E_F} D_{2D}(E) dE \quad (T = 0 \text{ K})$$
ECE 656 Homework 2: (Week 2) (continued)

\[ n_s = \frac{E_F}{\pi h^2 v_F^2} \]

\[ n_s = \frac{E_F^2}{\pi h^2 v_F^2} \]

1b) In terms of the Fermi wave vector, \( k_F \):

Case i): parabolic energy bands: DOS:

\[ \frac{h^2 k^2}{2m^*} = E - E_C = E \quad (E > E_C = 0) \]

\[ \frac{h^2 k_F^2}{2m^*} = E_F - E_C = E_F \quad (E > E_C = 0) \]

\[ n_s = \frac{2m^*}{\pi h^2} E_F \rightarrow n_s = \frac{2m^*}{\pi h^2} \times \frac{h^2 k_F^2}{2m^*} = g_v \times \frac{k_F^2}{2\pi} \]

\[ n_s = g_v \times \frac{k_F^2}{2\pi} \]

Case ii): graphene: DOS:

\[ E = \hbar v_F k \quad (E > 0) \]

\[ E_F = \hbar v_F k_F \quad (E_F > 0) \]

\[ n_s = \frac{E_F^2}{\pi h^2 v_F^2} \rightarrow \frac{(\hbar v_F k_F)^2}{\pi h^2 v_F^2} = \frac{k_F^2}{\pi} \]

\[ n_s = \frac{k_F^2}{\pi} \quad \text{(same as for parabolic energy bands)} \]

Aside: Why are the two expressions the same?

At \( T = 0 \) K, all of the states with \( k < k_F \) are occupied and all for \( k > k_F \) are empty. The area of occupied k-space is \( \pi k_F^2 \).

In 2D, each state occupies an area in k-space of \( (2\pi)^2 / A \)

So the number of states occupied is:
ECE 656 Homework 2: (Week 2) (continued)

\[ N = \frac{\pi k_F^2}{(2\pi)^2 / A} \times 2 \times g_v \]

where the factor of 2 is for spin degeneracy and \( g_v \) is the valley degeneracy. The sheet carrier density is

\[ n_s = \frac{N}{A} = \frac{k_F^2}{2\pi} \times g_v = \frac{k_F^2}{\pi} \] (because valley degeneracy is 2 for both cases consider here.)

2) Assume a finite temperature and work out the sheet carrier densities, \( n_s \), for:

2a) Electrons in the conduction band of a 2D parabolic band semiconductor

2b) Electrons in the conduction band \( (E > 0) \) of graphene.

Solution:

2a) parabolic energy bands

\[ n_s = \int_{E_c}^{\infty} D_{2D}(E) f_0(E) dE = \int_{E_c}^{\infty} \left( \frac{g_v m^*}{\pi \hbar^2} \right) \frac{1}{1 + e^{(E-E_F)/k_BT}} dE \]

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

define:

\[ \eta_F = \frac{E_F - E_C}{k_BT} \]

\[ \eta = \frac{E - E_C}{k_BT} \]

\[ d\eta = \frac{dE}{k_BT} \]

\[ dE = k_BT d\eta \]

with this change of variables, we find:

\[ n_s = \left( \frac{g_v m^*}{\pi \hbar^2} \right) \int_{0}^{\infty} k_BT d\eta \]

the integral can be done analytically:
ECE 656 Homework 2: (Week 2) (continued)

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

but we also recognize it as a Fermi-Dirac integral of order 0:

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

so the answer is:

\[
\begin{array}{l}
n_S = N_{2D} F_0(\eta_F) \\
N_{2D} = \frac{m^* k_B T}{\pi \hbar^2}
\end{array}
\]

2b) graphene

\[
n_S = \int_{E_c}^\infty D_{2D}(E) f_0(E) dE = \int_0^\infty \left( \frac{2E}{\pi \hbar^2 \nu_F^2} \right) \frac{1}{1 + e^{(E - E_c)/k_B T}} dE
\]

define:

\[
\eta_F = \frac{E_F}{k_B T} \quad \eta = \frac{E}{k_B T} \quad E = k_B T \eta \quad d\eta = \frac{dE}{k_B T} \quad dE = k_B T d\eta
\]

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

The integral is recognized as a Fermi-Dirac integral of order 1:

\[
n_S = \frac{2}{\pi} \left( \frac{k_B T}{\hbar \nu_F} \right)^2 \int_0^\infty \frac{\eta d\eta}{1 + e^{\eta - \eta_F}} = \frac{2}{\pi} \left( \frac{k_B T}{\hbar \nu_F} \right)^2 F_1(\eta_F)
\]

\[
\begin{array}{l}
n_S = N_{2D} F_1(\eta_F) \\
N_{2D} = \frac{2}{\pi} \left( \frac{k_B T}{\hbar \nu_F} \right)^2
\end{array}
\]
ECE 656 Homework 2: (Week 2) (continued)

3) Assume $T = 0$K and work out the average $+x$-directed velocity for electrons in:

3a) A 2D semiconductor with a parabolic conduction band and

3b) The conduction band ($E > 0$) of graphene.

Your answer should be in terms of the Fermi energy, $E_F$.

Solution:

3a) parabolic energy bands

$$\langle v_x^+ \rangle = \frac{\sum_{k_x > 0} v_x(\vec{k}) f_0(E)}{\sum_{k_x > 0} f_0(E)} = \frac{\int \int \frac{h k}{m} \cos \theta f_0}{\int \int k dk d\theta f_0}$$

(DOS in $k$-space cancels from num and denom)

$$\text{num} = \int \int k dk d\theta f_0 = \int \int k dk d\theta \frac{h k}{m} \cos \theta f_0$$

$f_0 = 1 \quad k < k_F \quad (E < E_F)$

$$\text{num} = \int \int k dk d\theta \frac{h k}{m} \cos \theta = \frac{h}{m} \int k dk \int \cos \theta d\theta = \frac{h}{m} \left( \frac{k_F^3}{3} \right) \times 2$$

$$\text{num} = \left( \frac{2}{3} \right) \left( \frac{h k_F^3}{m^*} \right) \quad (*)$$

$$\text{denom} = \int \int k dk d\theta f_0 = \int \int k dk d\theta = \int k dk \int d\theta = \frac{k_F^2}{2} \times \pi \quad (***)$$

Using (*) and (***)

$$\langle v_x^+ \rangle = \frac{\text{num}}{\text{denom}} = \left( \frac{2}{3} \right) \left( \frac{h k_F^3}{m^*} \right) = \frac{4}{3\pi} \frac{h k_F}{m} = \frac{4}{3\pi} v_F$$
ECE 656 Homework 2: (Week 2) (continued)

\[ \left\langle v_x^+ \right\rangle = \frac{4}{3\pi} v_F \]

Makes sense….. ave. x-directed velocity must be less than the maximum velocity of electrons in the conduction band, \(v_F\).

3b) graphene

\[ \left\langle v_x^+ \right\rangle = \frac{\sum_{k_x > 0, k_y} v_x(\vec{k}) f_0(E)}{\sum_{k_x > 0, k_y} f_0(E)} = \frac{\int_{0}^{\infty} \int_{-\pi/2}^{\pi/2} k dk d\theta v_x f_0}{\int_{0}^{\infty} \int_{-\pi/2}^{\pi/2} k dk d\theta f_0} \]

\[ \text{num} = \int_{0}^{\infty} \int_{-\pi/2}^{\pi/2} k dk d\theta v_x f_0 = \int_{0}^{\infty} \int_{0}^{\pi/2} k dk d\theta v_x \cos \theta f_0 \]

\[ f_0 = 1 \quad k < k_F (E < E_F) \]

\[ \text{num} = \int_{0}^{k_F} \int_{-\pi/2}^{\pi/2} k dk d\theta \cos \theta = v_F \int_{0}^{k_F} \int_{0}^{-\pi/2} \cos \theta d\theta = v_F \left( \frac{k_F^2}{2} \right) \times 2 \]

\[ \text{num} = v_F k_F^2 \quad (*) \]

\[ \text{den} = \int_{0}^{\infty} \int_{-\pi/2}^{\pi/2} k dk d\theta f_0 = \int_{0}^{\infty} \int_{0}^{\pi/2} k dk d\theta = \int_{0}^{k_F} \int_{0}^{\pi/2} d\theta = \frac{k_F^2}{2} \times \pi \quad (**) \]

From (*) and (**), we find:

\[ \left\langle v_x^+ \right\rangle = \frac{\text{num}}{\text{den}} = \frac{v_F k_F^2}{k_F^2 \pi / 2} = \frac{2}{\pi} v_F \]

\[ \left\langle v_x^+ \right\rangle = \frac{2}{\pi} v_F \]
ECE 656 Homework 2: (Week 2) (continued)

4) Assume a nonparabolic, 1D energy bandstructure described by:

\[ E(k_x)[1 + \alpha E(k_x)] = \frac{\hbar^2 k_x^2}{2m^*(0)} \]

where

\[
\frac{1}{m^*(0)} = \left. \frac{1}{\hbar^2} \frac{d^2 E(k_x)}{dk_x^2} \right|_{k_x=0}.
\]

4a) Sketch (or produce a Matlab plot) of \( E(k) \) vs. \( k \) for two cases: i) \( \alpha = 0 \) and ii) \( \alpha > 0 \). If you are producing a Matlab plot, the energy range should be from 0 to 1 eV, and you can assume \( \alpha = 0.5 \) eV.

**Solution:**

We can see from the equation, that for a given \( E \), the left hand side will be bigger than for a parabolic energy band, so it will take a bigger \( k_x \) for that \( E \). The bands flatten out as shown below.

![Graph showing energy-bandstructure](image)

4b) For this bandstructure, derive an expression for the velocity, \( v_x(k_x) \) as a function of \( k_x \).

**Solution:**

Velocity is related to bandstructure by:

\[ v_x = \frac{1}{\hbar} \frac{dE}{dk_x} \]
ECE 656 Homework 2 (Week 2) (continued)

\[ E + \alpha E^2 = \frac{\hbar^2 k_x^2}{2m^*(0)} \]

\[ \frac{dE}{dk_x} + 2\alpha E \frac{dE}{dk_x} = \frac{\hbar^2 k_x}{m^*(0)} \]

\[ \frac{dE}{dk_x}(1 + 2\alpha E) = \frac{\hbar^2 k_x}{m^*(0)} \]

\[ \frac{1}{\hbar} \frac{dE}{dk_x} = \frac{1}{\hbar} \frac{\hbar^2 k_x}{m^*(0)(1 + 2\alpha E)} = v_x \]

\[ v_x = \frac{\hbar k_x}{m^*(0)(1 + 2\alpha E)} \]

alternatively, we could define an energy dependent effective mass by:

\[ m^*(E) = m^*(0)(1 + 2\alpha E) \]

and write the velocity as

\[ v_x = \frac{\hbar k_x}{m^*(E)} \]

5) For parabolic energy bands, the 2D density of states is

\[ D_{2D}(E) = \frac{m^*}{\pi \hbar^2} \Theta(E - \epsilon_1) \]

Assume a non-parabolic band described by the so-called Kane dispersion,

\[ E(k)[1 + \alpha E(k)] = \frac{\hbar^2 k^2}{2m^*(0)} \]

and derive the density of states.
Solution:

First, find the number of states in 2D k-space:

\[
N(k)dk_xdk_y = \left( \frac{A}{(2\pi)^2} \times 2 \right) 2\pi kdk = \frac{A}{2\pi} 2\pi kdk = \frac{A}{\pi} kdk
\]

Note that \( N(k)dk_xdk_y \) is the number of states per unit area. Now map these states onto energy:

\[
D_{2D}(E) dE = \frac{1}{A} N(k) dk = \frac{1}{\pi} kdk
\]

Note that by convention, \( D_{2D}(E) dE \) is the number of states per unit area. Solve for \( D_{2D}(E) \):

\[
D_{2D}(E) = \frac{1}{A} N(k) \frac{dk}{dE} = \frac{1}{\pi} k \frac{dk}{dE}
\] (*)

The bandstructure is:

\[
E + \alpha E^2 = \frac{\hbar^2 k^2}{2m^*(0)}
\]

Differentiate with respect to \( k \):

\[
1 + 2\alpha E = \frac{\hbar^2}{m^*(0)} k \frac{dk}{dE}
\]

\[
k \frac{dk}{dE} = \frac{m^*(0)}{\hbar^2} (1 + 2\alpha E)
\] (**)

Now insert (** into (*) to find:

\[
D_{2D}(E) = \frac{m^*(0)}{\pi \hbar^2} (1 + 2\alpha E)
\]
ECE 656 Homework 2 (Week 2) (continued)

6) Derive an expression for the 2D density of states for one of the conduction band ellipsoids in silicon.

HINT: You may find the discussion in Pierret (Advanced Semiconductor Fundamentals) on pp. 94-95 helpful.

Solution:

In this case, we write $E(k_x, k_y)$ as:

$$E = \frac{\hbar^2 k_x^2}{2m_{xx}^*} + \frac{\hbar^2 k_y^2}{2m_{yy}^*}$$

For the case shown, $m_{xx}^*$ is the longitudinal effective mass and $m_{yy}^*$ is the transverse effective mass.

Re-write $E = \frac{\hbar^2 k_x^2}{2m_{xx}^*} + \frac{\hbar^2 k_y^2}{2m_{yy}^*}$ as $E = \frac{\hbar^2 k_x^2}{2m_0} \left[ \left( \sqrt{\frac{m_0}{m_{xx}^*}} k_x \right)^2 + \left( \sqrt{\frac{m_0}{m_{yy}^*}} k_y \right)^2 \right]$

Now define a “stretched” k-space:

$$\tilde{k}_x = \sqrt{\frac{m_0}{m_{xx}^*}} k_x \quad \quad \tilde{k}_y = \sqrt{\frac{m_0}{m_{yy}^*}} k_y$$
ECE 656 Homework 2 (Week 2) (continued)

Now we can write the $E(k)$ in the stretched $k$-space:

$$E(\tilde{k}_x, \tilde{k}_y) = \frac{\hbar^2}{2m_0} \left( \tilde{k}_x^2 + \tilde{k}_y^2 \right) = \frac{\hbar^2 \tilde{k}_x^2}{2m_0}, \quad (*)$$

which looks like a simple, circular band in 2D. But we must realize that states are spaced $\left( 2\pi/L_x \right) \times \sqrt{m_0/m_{xx}}$ in $k_x$, but they are spaced $2\pi L_x \times m_{yy}$ in $\tilde{k}_x$. Accordingly, we find

$$N(k)dk_xdk_y = \frac{A}{(2\pi)^2} \times 2 \times \sqrt{\frac{m_{xx}m_{yy}}{m_0}} \tilde{k}_x \tilde{k}_y = \frac{A}{2\pi^2} \sqrt{\frac{m_{xx}m_{yy}}{m_0}} 2\pi \tilde{k}d\tilde{k} = \frac{A}{\pi} \sqrt{\frac{m_{xx}m_{yy}}{m_0}} \tilde{k}d\tilde{k}$$

$$D_{2D}(E)dE = \frac{1}{A} N(k)dk_xdk_y = \frac{1}{\pi} \sqrt{\frac{m_{xx}m_{yy}}{m_0}} \tilde{k} \frac{d\tilde{k}}{dE}$$

or, solving for the DOS:

$$D_{2D}(E) = \frac{1}{\pi} \sqrt{\frac{m_{xx}m_{yy}}{m_0}} \frac{d\tilde{k}}{dE} \quad (***)$$

Now use (*) to find:

$$\tilde{k} \frac{d\tilde{k}}{dE} = \frac{m_0}{\hbar^2}$$

and insert this in (**) to find

$$D_{2D}(E) = g_v \frac{m_0}{\pi \hbar^2} \sqrt{m_{xx}m_{yy}} = g_v \sqrt{\frac{m_{xx}m_{yy}}{\pi \hbar^2}}$$

For the primed valleys of Si, $m_{xx}^* = m_{yy}^*$ is the longitudinal effective mass and $m_{yy}^* = m_{xx}^*$ is the transverse effective mass. The valley degeneracy of the primed valleys is $g_v = 4$. Accordingly, for the primed valleys (of (100) Si), we find

$$D'_{2D}(E) = g_v \frac{\sqrt{m_{xx}m_{yy}}}{\pi \hbar^2} = \frac{4 \sqrt{m_{xx}m_{yy}}}{\pi \hbar^2},$$
ECE 656 Homework 2 (Week 2) (continued)

which can be written as

\[
\begin{align*}
D'_2(E, m^*_D) &= \frac{m^*_D}{\pi \hbar^2} \\
m^*_D &= 4\sqrt{m^*_r m^*_s}
\end{align*}
\]

The quantity, \( m^*_D \), is called the “density-of-states effective mass.”

7) Assume an ultra thin body (100) silicon structure with a thickness of 3 nm. Assume no bandbending within the structure and infinitely high energy barriers at the oxide-silicon interfaces. Compute and plot the 2D density of states vs. energy.

Solution:

The constant energy surfaces for Si are shown below. The “confinement mass” is the mass in the direction of confinement (assume z-direction) and the DOS effective masses are determined by the masses in the x-y plane.

Unprimed valleys:

\[
de_n = \frac{\hbar^2 n^2 \pi^2}{2m^*_r \ell^2_{Si}} \quad D'_2 = g_v \frac{m^*_r}{\pi \hbar^2} \quad g_v = 2
\]

Primed valleys:

\[
de'_n = \frac{\hbar^2 m^2 \pi^2}{2m^*_r \ell^2_{Si}} \quad D'_{2D} = g'_v \frac{\sqrt{m^*_r m^*_s}}{\pi \hbar^2} \quad g'_v = 4
\]

See the figures below:
specific numbers: unprimed valleys:

\[ \epsilon_n = \frac{\hbar^2 n^2 \pi^2}{2m_i^* t_{Si}^2} = \left( \frac{0.042}{m_i^*/m_0} \right) n^2 \text{ (eV)} \]

\[ \epsilon_1 = 0.046 \quad \epsilon_2 = 0.185 \quad \epsilon_3 = 0.415 \quad \epsilon_4 = 0.739 \]

\[ D_{2D} = g_v \frac{m_i^*}{\pi \hbar^2} = 0.38 \frac{m_0}{\pi \hbar^2} \]

\[ \frac{m_0}{\pi \hbar^2} = 4.2 \times 10^{14} \text{ (eV-cm}^2\text{)}^{-1} \]

specific numbers primed valleys:

\[ \epsilon'_n = \frac{\hbar^2 m^2 \pi^2}{2m_i^* t_{Si}^2} = \left( \frac{0.042}{m_i^*/m_0} \right) m^2 \text{ (eV)} \]

\[ \epsilon'_1 = 0.221 \quad \epsilon'_2 = 0.884 \quad \epsilon'_3 = 1.989 \quad \epsilon'_4 = 3.54 \]

Note that these are unreasonably large energies (especially for \( m > 1 \)) – due to the assumption of infinite barriers and parabolic energy bands.

\[ D_{2D} = g_v \sqrt{m_i^* m_0^*} \frac{m_0}{\pi \hbar^2} = 1.66 \]
ECE 656 Homework 2 (Week 2) (continued)

With this information, we can plot the DOS for the first few levels....