1) We have discussed $M(E)$ for a 3D semiconductor with parabolic energy bands. Answer the following two questions about a 3D semiconductor with non-parabolic energy bands.

a) Assume that the non-parabolicity can be described by

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

Derive an expression for the corresponding $M(E)$.

b) Using the following numbers for GaAs,

$m^*(0) = 0.067 m_0$

$\alpha = 0.64$,

plot $M(E)$ from the bottom of the $\Gamma$ valley to $E = 0.3$ eV comparing results from the non-parabolic expression derived in part a) to the parabolic expression.

Solutions:

We know that non-parabolicity flattens the bands – it increases the DOS and lowers the velocity, so it is not obvious whether $M(E)$ will be larger or smaller, since $M(E)$ is the product of the DOS and velocity. Let’s work it out and see what the answer is.

1a)

Begin with the definition:

$$M_{3D}(E) = \frac{\hbar}{4} \langle v_s^+ \rangle D_{3D}(E) \quad (1)$$

$$\langle v_s^+ \rangle = (1/2)v(E) \quad (2)$$

Step 1: compute $D_{3D}(E)$ for non-parabolic bands
Step 2: compute $v(E)$ for non-parabolic bands
Step 3: multiply the two to get the answer
ECE 656 Homework (Week 6) Solutions  (continued)

Step 1:

\[ D_{3D}(E) dE = \frac{N_{3D}(k)}{\Omega} 4\pi k^2 dk = \frac{1}{\frac{4\pi^3}{3} 4\pi k^2} dk = \frac{1}{\pi^2} k^2 dk \]  

(3)

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

(4)

Solve for \(k\):

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

(5)

differentiate to find:

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

(6)

put the two together:

\[ k^2 dk = \frac{m^*(0)}{\hbar^3} \sqrt{2m^*(0)E(1+\alpha E)(1+2\alpha E)} dE \]

Insert in (3)

\[ D_{3D}(E) dE = \frac{1}{\pi^2} k^2 dk = \frac{m^*(0)}{\pi^2 \hbar^3} \sqrt{2m^*(0)E(1+\alpha E)(1+2\alpha E)} dE \]

\[ D_{3D}(E) = \frac{1}{\pi^2} k^2 dk = \frac{m^*(0)}{\pi^2 \hbar^3} \sqrt{2m^*(0)E(1+\alpha E)(1+2\alpha E)} \]  

(7)

Step 2:

From (6)

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

Now use (5)

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

(8)
ECE 656 Homework (Week 6) Solutions (continued)

Step 3:
Now use (1), (2), (7), and (8)

\[
M_{3D}(E) = \frac{h}{4}\left(\frac{\nu(E)}{2}\right)D_{3D}(E) = \frac{h}{4}\left(\frac{\nu(E)}{2}\right)D_{3D}(E) = \frac{h}{4}\sqrt{E(1+\alpha E)} \left(\frac{1}{2m^*(0)} - \frac{1}{(1+2\alpha E)}\right)D_{3D}(E)
\]

\[
M_{3D}(E) = \frac{h}{4}\sqrt{\frac{E(1+\alpha E)}{2m^*(0)}} \left(\frac{1}{1+2\alpha E}\right)\left[\frac{m^*(0)}{\pi^2h^3} \sqrt{2m^*(0)E(1+\alpha E)(1+2\alpha E)}\right]
\]

\[
M_{3D}(E) = \frac{m^*(0)}{2\pi h^2}E(1+\alpha E)
\]

We have been assuming that the bottom of the conduction band is at \(E_C = 0\). Let's put \(E_C\) back in explicitly.

\[
M_{3D}(E) = \frac{m^*(0)}{2\pi h^2}(E-E_C)[1+\alpha(E-E_C)]
\]

So we see that the \(M(E)\) increases when the bands are nonparabolic.

1b) The following Matlab script is used to produce the plot below.

```matlab
gset(get(gca, 'ylabel'), 'FontSize', font_size);
```

![Graph showing non-parabolic and parabolic behaviors of M(E) vs. Energy (eV)]
function ece656_hw6_1b()

% ECE 656 (Fall 2013) HW#6, 1b
% This script plots and compares the density of modes for GaAs assuming parabolic
% and non-parabolic energy bands

m_star = 0.067; % (1) effective mass coefficient
alpha = 0.64; % (/eV) non-parabolicity factor
m_o = 0.511e6; % (eV/c^2) electron rest mass
hbar = 6.582e-16; % (eV-s)
m = m_star*m_o; % (eV/c^2) electron effective mass
E = linspace(0,0.3,100); % (eV) range of energy

Calculation of Modes

M_3D_nonp = m./(2*pi*hbar^2).*E.*(1+alpha.*E).*1e-4; % (/cm^2)
M_3D_p = m./(2*pi*hbar^2).*E.*1e-4; % (/cm^2)

Plots

figure(1)
plot(E, M_3D_nonp,'LineWidth',2)
hold on
plot(E, M_3D_p,'--','LineWidth',2)
xlabel('Energy (eV)');
ylabel('M(E) (/cm^2)');
legend('Non-parabolic','Parabolic','Location','NorthWest');
xlim([0 max(E)])

font_size = 12;
set(gcf, 'color', 'white');
set(gca, 'FontSize',font_size);
set(get(gca,'title'),'FontSize',font_size);
set(get(gca,'xlabel'),'FontSize',font_size);
set(get(gca,'ylabel'),'FontSize',font_size);
2) The figure below shows a semiconductor with the Fermi level located in five different locations. If we use the Landauer expression to compute the current:

$$ I = \frac{2q}{h} \int_{E_1}^{E_2} T(E) M(E)(f_1 - f_2) dE $$

what are appropriate limits of integration, $E_1$ and $E_2$, for each case? You may assume room temperature, a bandgap of 1 eV, and that $E_{F1} = E_{F2} = E_F$.

Solution:

**Case 1:** Only states in the conduction band are involved, so

$$ I = \frac{2q}{h} \int_{E_C}^{\infty} T(E) M(E)(f_1 - f_2) dE $$

We could safely replace $\infty$ with $E_F + 5k_B T$.

**Case 2:** Again, only states in the conduction band are involved, so

$$ I = \frac{2q}{h} \int_{E_C}^{E_1} T(E) M(E)(f_1 - f_2) dE $$

We could safely replace $\infty$ with $E_C + 5k_B T$. 
ECE 656 Homework (Week 6) Solutions (continued)

**Case 3:** There are not many electrons or holes involved, but we need to include both bands.

\[
I = \left(\frac{2q}{h}\right) \int_{-\infty}^{+\infty} T(E) M(E) (f_1 - f_2) dE
\]

We could safely replace \(+\infty\) with \(E_C + 5k_B T\) and \(-\infty\) with \(E_v - 5k_B T\).

**Case 4:** Only states in the valence band are involved, so

\[
I = \left(\frac{2q}{h}\right) \int_{-\infty}^{E_v} T(E) M(E) (f_1 - f_2) dE
\]

We could safely replace \(-\infty\) with \(E_v - 5k_B T\).

**Case 5:** Again, only states in the valence band are involved, so

\[
I = \left(\frac{2q}{h}\right) \int_{E_F}^{E_v} T(E) M(E) (f_1 - f_2) dE
\]

We could safely replace \(-\infty\) with \(E_F - 5k_B T\).

3) Determine the limits of integration, \(E_1\) and \(E_2\), for the integral in the Landauer expression:

\[
I = \left(\frac{2q}{h}\right) \int_{E_1}^{E_2} T(E) M(E) (f_1 - f_2) dE
\]

for the case of \(T = 0\) K. Assume that contact one is grounded and that a positive voltage (not necessarily small) has been applied to contact 2.

**Solution:**

In the left contact, states below \(E_{F1}\) are occupied, and in the right contact, states below \(E_{F2} = E_{F1} - qV\) are occupied. The only ranges where \((f_1 - f_2)\) is \(E_{F2} < E < E_{F1}\), so

\[
I = \left(\frac{2q}{h}\right) \int_{E_{F2}}^{E_{F1}} T(E) M(E) (f_1 - f_2) dE
\]
4) The ballistic conductance is often derived from a k-space treatment, which writes the current from left to right as

$$I^+ = \frac{1}{L} \sum_{k>0} q v_x f_0(E_{F_1})$$

and the current from right to left as

$$I^- = \frac{1}{L} \sum_{k<0} q v_x f_0(E_{F_2})$$

The net current is the difference between the two. In the ballistic limit, the Landauer expression for the current is

$$I = (2q/h) \int_{E_1}^{E} M(E) (f_1 - f_2) dE$$

4a) Assume parabolic energy bands, evaluate the net current from the k-space approach, and show that it is the same as the Landauer expression.

**Solution:**

$$I^+ = \frac{1}{L} \sum_{k>0} q v_x f_0(E_{F_1}) = \frac{1}{L} \frac{L}{2\pi} \times 2 \int_0^{\infty} q f_0(E_{F_1}) dk$$

$$I^- = \frac{q}{\pi} \times \int_0^{\infty} f_0(E_{F_1}) dk = \frac{q}{\pi} \int_0^{\infty} f_0(E_{F_1}) \frac{dk}{dE} dE$$

$$E = \frac{\hbar^2 k^2}{2m^*} \quad dE = \frac{\hbar^2 dk}{m^*} \quad dk = \frac{m^* dE}{\hbar^2 k} \quad k = \sqrt{\frac{2m^* E}{\hbar}} \quad \frac{dk}{dE} = \frac{m^*}{\hbar \sqrt{2m^* E}} = \frac{1}{\hbar} \sqrt{\frac{m^*}{2E}}$$

$$I^+ = q \int_0^{\infty} \sqrt{\frac{m^*}{2E}} f_0(E_{F_1}) dE$$

$$I^- = \frac{2q}{h} \int_0^{\infty} \frac{2}{4} \sqrt{\frac{m^*}{2E}} f_0(E_{F_1}) dE = \frac{2q}{h} \int_0^{\infty} \left\{ \frac{h}{4} \nu D_i(E) \right\} f_0(E_{F_1}) dE$$

$$I^+ = \frac{2q}{h} \int_0^{\infty} M(E) f_0(E_{F_1}) dE$$

where

$$M(E) \equiv \frac{h}{4} \langle \nu_i^+ \rangle D_i(E) \quad \langle \nu_i^+ \rangle = \nu$$
ECE 656 Homework (Week 6) Solutions (continued)

Similarly, we can show:

\[ I^- = \frac{2q}{\hbar} \int_{0}^{\infty} M(E) f_0(E_{F_2}) dE \]

The net current is

\[ I = I^+ - I^- = \frac{2q}{\hbar} \int_{0}^{\infty} M(E) \left[ f_0(E_{F_1}) - f_0(E_{F_2}) \right] dE \]

\[ I = \frac{2q}{\hbar} \int_{0}^{\infty} M(E)(f_1 - f_2) dE \]

Note that in solving this problem, we have also defined \( M(E) \) and \( \langle v^+_x \rangle \) in 1D with parabolic energy bands.

4b) Assume parabolic energy bands, but now assume 2D electrons. Evaluate the net current from the k-space approach, and show that it is the same as the Landauer expression.

**Solution:**

\[ I^+ = \frac{1}{A} \sum_{k_x > 0} q v_x f_0(E_{F_1}) = \frac{1}{A (2\pi)^2} \times 2 \int_{\theta}^{\pi/2} \int_{0}^{\infty} q v \cos \theta f_0(E_{F_1}) k dk d\theta \]

\[ \int_{-\pi/2}^{\pi/2} \cos \theta d\theta = 2 \]

\[ I^+ = \frac{q}{2\pi^2} \int_{0}^{\infty} 2v f_0(E_{F_1}) k dk = \frac{q}{2\pi^2} \int_{0}^{\infty} 2v f_0(E_{F_1}) \frac{k dk}{dE} dE \]

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

\[ I^+ = \frac{q}{2\pi} \int_{0}^{\infty} 2v f_0(E_{F_1}) \left( \frac{m^*}{\pi^2 \hbar^2} \right) dE = \frac{q}{2} \int_{0}^{\infty} \langle v_x^+ \rangle f_0(E_{F_1}) D_{2D} dE \]

where

\[ \langle v_x^+ \rangle = \frac{2}{\pi} \nu \]
ECE 656 Homework (Week 6) Solutions (continued)

\[ I^+ = \frac{q}{2} \int_0^{+\infty} \langle \psi^*_i \rangle D_{2D} f_0(E_{F_1}) dE = I^+ = \frac{2q}{\hbar} \int_0^{+\infty} \left( \frac{\hbar}{4} \langle \psi^*_i \rangle D_{2D} \right) f_0(E_{F_1}) dE \]

\[ I^+ = \frac{2q}{\hbar} \int_0^{+\infty} M(E) f_0(E_{F_1}) dE \]

where

\[ M(E) = \frac{\hbar}{4} \langle \psi^*_i \rangle D_{2D}(E) \]

Similarly, we can show:

\[ I^- = \frac{2q}{\hbar} \int_0^{+\infty} M(E) f_0(E_{F_2}) dE \]

The net current is

\[ I = I^+ - I^- = \frac{2q}{\hbar} \int_0^{+\infty} \left[ f_0(E_{F_1}) - f_0(E_{F_2}) \right] dE \]

\[ I = \frac{2q}{\hbar} \int_0^{+\infty} M(E) f_0(E_{F_1}) - f_0(E_{F_2}) dE \]

Note that in solving this problem, we have also defined \( M(E) \) and \( \langle \psi^*_i \rangle \) in 2D with parabolic energy bands.

4c) Assume parabolic energy bands, but now assume 3D electrons. Evaluate the net current from the k-space approach, and show that it is the same as the Landauer expression.

Solution:

\[ I^+ = \frac{1}{\Omega} \sum_{k_x > 0} qv_x f_0(E_{F_1}) = \frac{1}{\Omega} \left( \frac{\Omega}{2\pi} \right)^3 \times 2 \int_0^{+\infty} \int_0^{-\pi/2} qv \sin \theta \cos \phi f_0(E_{F_1}) k^2 \sin \theta d\theta d\phi dk \]

\[ I^+ = \frac{q}{4\pi^3} \int_0^{+\pi/2} \int_0^{-\pi/2} v \sin \theta \cos \phi f_0(E_{F_1}) k^2 \sin \theta d\theta d\phi dk \]

\[ \int_{-\pi/2}^{+\pi/2} \cos \phi d\phi = 2 \]
ECE 656 Homework (Week 6) Solutions (continued)

\[ I^* = \frac{q}{2\pi^2} \int \int_0^{\pi} \sin \theta f_0(E_{F_1}) k^2 \sin \theta d\theta dk \]

\[ \int_0^\pi \sin^2 \theta d\theta = \frac{\pi}{2} \]

\[ I^* = \frac{q}{4\pi^2} \int_0^\pi \psi f_0(E_{F_1}) k^2 dk = \frac{q}{4\pi^2} \int_0^\pi \psi f_0(E_{F_1}) k^2 \frac{dk}{dE} dE \]

\[ E = \frac{\hbar^2 k^2}{2m^*} \quad dE = \frac{\hbar^2 k dk}{m^*} \quad k dk = \frac{m^* dE}{\hbar^2} \quad k = \frac{\sqrt{2m^* E}}{\hbar} \]

\[ k^2 dk = \frac{\sqrt{2m^* E} m^* dE}{\hbar^2} = \frac{m^* \sqrt{2m^* E}}{\hbar^3} dE \]

\[ I^* = \frac{q}{4\pi^2} \int_0^\pi \psi f_0(E_{F_1}) \frac{dk}{dE} dE = \frac{q}{4\pi^2} \int_0^\pi \psi f_0(E_{F_1}) \frac{m^* \sqrt{2m^* E}}{h^3} dE \]

\[ I^* = \frac{q}{4} \int_0^\infty \left( \frac{m^* \sqrt{2m^* E}}{\pi^2 \hbar^3} \right) f_0 \left( E_{F_1} \right) dE \]

\[ I^* = \frac{q}{2} \int_0^\infty \left( \frac{\hbar}{4} \langle \psi_x^+ \rangle D_{3D}(E) \right) f_0 \left( E_{F_1} \right) dE \]

where

\[ \langle \psi_x^+ \rangle = \frac{\psi}{2} \]

\[ I^* = \frac{2q}{h} \int_0^\infty \left( \frac{\hbar}{4} \langle \psi_x^+ \rangle D_{3D}(E) \right) f_0 \left( E_{F_1} \right) dE \]

\[ I^* = \frac{2q}{h} \int_0^\infty M \left( E \right) f_0 \left( E_{F_1} \right) dE \]

where

\[ M \left( E \right) = \frac{h}{4} \langle \psi_x^+ \rangle D_{3D}(E) \]
ECE 656 Homework (Week 6) Solutions (continued)

Similarly, we can show:

\[ I^- = \frac{2q}{\hbar} \int_{0}^{\infty} M(E) f_0(E_{F2}) dE \]

The net current is

\[ I = I^+ - I^- = \frac{2q}{\hbar} \int_{0}^{\infty} M(E) [f_0(E_{F1}) - f_0(E_{F2})] dE \]

\[ I = \frac{2q}{\hbar} \int_{0}^{\infty} M(E) (f_1 - f_2) dE \]

Note that in solving this problem, we have also defined \( M(E) \) and \( \langle \psi_+ \rangle \) in 3D with parabolic energy bands.

5) The quantity,

\[ \langle M \rangle = \int_{E_c}^{\infty} M(E) \left( -\frac{\partial f_0}{\partial E} \right) dE \]

is the number of conduction band channels in the Fermi-Window. Answer the following questions.

5a) Evaluate \( \langle M \rangle \) for an arbitrary temperature and location of the Fermi level assuming a 2D semiconductor with parabolic energy bands.

Solution:

\[ \langle M \rangle = \int_{E_c}^{\infty} M(E) \left( -\frac{\partial f_0}{\partial E} \right) dE = \frac{\partial}{\partial E_F} \int_{E_c}^{\infty} M(E) f_0(E) dE \]

\[ M(E) = W M_{2D}(E) = W \sqrt{2m^*(E - E_c)} \]

\[ \frac{\pi \hbar}{2m^*} \]
ECE 656 Homework (Week 6) Solutions (continued)

\[ \langle M \rangle = \frac{\partial}{\partial E_F} \int_{E_C}^{\infty} \frac{2m^*(E - E_C)}{\pi \hbar} \frac{1}{1 + e^{(E - E_F)/k_BT}} dE \]

\[ \langle M \rangle = W \frac{\sqrt{2m^*\pi \hbar}}{\sqrt[3]{4\pi}} \frac{\partial}{\partial E_F} \int_{E_C}^{\infty} \sqrt{E - E_C} \frac{1}{1 + e^{(E - E_F + E_C - E_F)/k_BT}} dE \]

\[ \langle M \rangle = W \frac{\sqrt{2m^*\pi \hbar}}{\sqrt[3]{4\pi}} \frac{\partial}{\partial \eta} \int_{0}^{\infty} \frac{\sqrt{\eta}}{1 + e^{\eta - \eta_F}} d\eta \]

where

\[ \eta = \frac{E - E_C}{k_BT} \text{ and } \eta_F = \frac{E_F - E_C}{k_BT} \]

\[ \langle M \rangle = W \frac{\sqrt{2m^*\pi \hbar}}{\sqrt[3]{4\pi}} \frac{1}{k_BT} \left[ \frac{\sqrt{\pi}}{2} F_{1/2} (\eta_F) \right] = W \frac{m^*}{\sqrt[3]{2\pi \hbar}} \frac{1}{k_BT} \left( k_BT \right)^{1/2} F_{-1/2} (\eta_F) \]

\[ \langle M \rangle = W \frac{\sqrt{2m^*\pi \hbar}}{\sqrt[3]{4\pi}} \frac{1}{k_BT} \left( k_BT \right)^{1/2} F_{-1/2} (\eta_F) \]

5b) Evaluate \( \langle M \rangle \) for an arbitrary temperature and location of the Fermi level above the Dirac point, \( E_D \), assuming graphene.

**Solution:**

The DOS is:

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

\[ M(E) = W \frac{h}{4} \left( v_F^* \right) D_{2D}(E) = W \frac{h}{4} \left( \frac{2(E - E_D)}{\pi h^2 v_F^2} \right) = W \frac{4}{v_F} \left( E - E_D \right) \]

\[ \langle M \rangle = \int_{E_D}^{\infty} M(E) \left( -\frac{\partial f_0}{\partial E} \right) dE = \frac{\partial}{\partial E_F} \int_{E_D}^{\infty} M(E) f_0(E) dE \]

\[ \langle M \rangle = W \frac{4}{v_F} \frac{\partial}{\partial E_F} \int_{E_D}^{\infty} \left( E - E_D \right) \frac{1}{1 + e^{(E - E_F)/k_BT}} dE \]

\[ \langle M \rangle = W \frac{4}{v_F} \left( k_BT \right)^{1/2} \frac{\partial}{\partial \eta} \int_{0}^{\infty} \frac{\eta}{1 + e^{\eta - \eta_F}} d\eta \]

\[ \langle M \rangle = W \frac{4}{v_F} \left( k_BT \right)^{1/2} \frac{\partial}{\partial \eta} F_{1/2} (\eta_F) \]
ECE 656 Homework (Week 6) Solutions (continued)

\[ \langle M \rangle = W \frac{4}{v_F h} (k_B T) F_0 (\eta_F) \]

5c) Assume that \( E_F = E_C + 0.1 \text{ eV} = E_D + 0.1 \text{ eV} \). For 5a), assume Si with \( m^* = 0.19 m_0 \) and a valley degeneracy of 2. For 5b), assume graphene parameters, \( v_F = 10^8 \text{ cm/s} \) and a valley degeneracy of 2. Compare the numerical values of \( \langle M \rangle \) for these two cases assuming \( T = 300 \text{ K} \).

Solution:

\[
\frac{\langle M \rangle_{\text{Si}}}{\langle M \rangle_{\text{graphene}}} = \frac{g_F W \sqrt{\frac{m^*}{2 \pi} \frac{1}{h} (k_B T)^{1/2} F_{-1/2}(\eta_F)}}{g_F W \frac{4}{v_F h} (k_B T) F_0 (\eta_F)}
\]

\[
\frac{\langle M \rangle_{\text{Si}}}{\langle M \rangle_{\text{graphene}}} = \frac{v_F}{2} \sqrt{\frac{\pi m^*}{2 k_B T}} \left( \frac{F_{-1/2}(\eta_F)}{F_0(\eta_F)} \right)
\]

\[
\frac{\langle M \rangle_{\text{Si}}}{\langle M \rangle_{\text{graphene}}} = \frac{v_F}{2 v_T} \left( \frac{F_{-1/2}(\eta_F)}{F_0(\eta_F)} \right)
\]

where

\[ v_T = \sqrt{\frac{2 k_B T}{\pi m^*}} = 1.23 \times 10^7 \text{ cm/s} \]

\[
\frac{\langle M \rangle_{\text{Si}}}{\langle M \rangle_{\text{graphene}}} = \frac{10^8}{2.47 \times 10^7} \left( \frac{F_{-1/2}(\eta_F)}{F_0(\eta_F)} \right) = 4.05 \times \left( \frac{F_{-1/2}(\eta_F)}{F_0(\eta_F)} \right)
\]

\[ \eta_F = 0.1 / 0.026 = 3.85 \]

\[
\frac{\langle M \rangle_{\text{Si}}}{\langle M \rangle_{\text{graphene}}} = 4.05 \times \left( \frac{F_{-1/2}(3.85)}{F_0(3.85)} \right) = 4.05 \times \left( \frac{2.1392}{3.821} \right) = 2.27
\]

\[
\frac{\langle M \rangle_{\text{Si}}}{\langle M \rangle_{\text{graphene}}} = 2.27
\]