

SOLUTIONS: ECE 656 Homework 2 (Week 2)

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- 1) Assume $T = 0\text{K}$ 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:

$$D_{2D}(E) = g_V \frac{m^*}{\pi \hbar^2} = \frac{2m^*}{\pi \hbar^2} \quad (E > E_C = 0)$$

$$n_S = \int_{E_C}^{\infty} D_{2D}(E) f_0(E) dE = n_S = \int_0^{E_F} D_{2D}(E) 1 dE \quad (T = 0 \text{ K})$$

$$n_S = \int_0^{E_F} g_V \frac{m^*}{\pi \hbar^2} dE = 2 \frac{m^*}{\pi \hbar^2} E_F$$

$$\boxed{n_S = g_V \frac{m^*}{\pi \hbar^2} E_F = \frac{2m^*}{\pi \hbar^2} E_F}$$

Case ii): graphene: DOS:

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

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!

$$n_S = \int_{E_C}^{\infty} D_{2D}(E) f_0(E) dE = n_S = \int_0^{E_F} D_{2D}(E) 1 dE \quad (T = 0 \text{ K})$$

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$$n_s = \int_0^{E_F} \frac{2E}{\pi \hbar^2 v_F^2} dE = \frac{E_F^2}{\pi \hbar^2 v_F^2}$$

$$n_s = \frac{E_F^2}{\pi \hbar^2 v_F^2}$$

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

Case i): parabolic energy bands: DOS:

$$\frac{\hbar^2 k^2}{2m^*} = E - E_C = E \quad (E > E_C = 0)$$

$$\frac{\hbar^2 k_F^2}{2m^*} = E_F - E_C = E_F \quad (E > E_C = 0)$$

$$n_s = \frac{2m^*}{\pi \hbar^2} E_F \rightarrow n_s = \frac{2m^*}{\pi \hbar^2} \times \frac{\hbar^2 k_F^2}{2m^*} = g_V \times \frac{k_F^2}{2\pi}$$

$$n_s = g_V \frac{k_F^2}{2\pi} = \frac{k_F^2}{\pi}$$

Case ii): graphene: DOS:

$$E = \hbar v_F k \quad (E > 0)$$

$$E_F = \hbar v_F k_F \quad (E_F > 0)$$

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

$$n_s = \frac{k_F^2}{\pi}$$

(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 πk_F^2

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

So the number of states occupied is:

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$$N = \frac{\pi k_F^2}{(2\pi)^2 / A} \times 2 \times g_V$$

where the factor of 2 is for spin degeneracy and g_V is the valley degeneracy. The sheet carrier density is

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

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**

$$n_s = \int_{E_C}^{\infty} D_{2D}(E) f_0(E) dE = \int_{E_C}^{\infty} \left(g_V \frac{m^*}{\pi \hbar^2} \right) \frac{1}{1 + e^{(E-E_F)/k_B T}} dE$$

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

define:

$$\eta_F = \frac{E_F - E_C}{k_B T} \quad \eta = \frac{E - E_C}{k_B T} \quad d\eta = \frac{dE}{k_B T} \quad dE = k_B T d\eta$$

with this change of variables, we find:

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

the integral can be done analytically:

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

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

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

so the answer is:

$$\boxed{n_S = N_{2D} \mathcal{F}_0(\eta_F)}$$

$$N_{2D} = g_v \frac{m^* k_B T}{\pi \hbar^2}$$

2b) graphene

$$n_S = \int_{E_C}^{\infty} D_{2D}(E) f_0(E) dE = \int_0^{\infty} \left(\frac{2E}{\pi \hbar^2 v_F^2} \right) \frac{1}{1 + e^{(E - E_F)/k_B T}} dE$$

define:

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

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

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

$$n_S = \frac{2}{\pi} \left(\frac{k_B T}{\hbar v_F} \right)^2 \int_0^{\infty} \frac{\eta d\eta}{1 + e^{\eta - \eta_F}} = \frac{2}{\pi} \left(\frac{k_B T}{\hbar v_F} \right)^2 \mathcal{F}_1(\eta_F)$$

$$\boxed{n_S = N_{2D} \mathcal{F}_1(\eta_F)}$$

$$N_{2D} = \frac{2}{\pi} \left(\frac{k_B T}{\hbar v_F} \right)^2$$

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3) Assume $T = 0\text{K}$ 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

$$\langle v_x^+ \rangle = \frac{\sum_{k_x > 0, k_y} v_x(\vec{k}) f_0(E)}{\sum_{k_x > 0, k_y} f_0(E)} = \frac{\int_0^{\infty} \int_{-\pi/2}^{+\pi/2} k dk d\theta v_x f_0}{\int_0^{\infty} \int_{-\pi/2}^{+\pi/2} k dk d\theta f_0} = \frac{\text{num}}{\text{den}} \quad (\text{DOS in k-space cancels from num and denom})$$

$$\text{num} = \int_0^{\infty} \int_{-\pi/2}^{+\pi/2} k dk d\theta v_x f_0 = \int_0^{\infty} \int_{-\pi/2}^{+\pi/2} k dk d\theta \frac{\hbar k}{m^*} \cos\theta f_0$$

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

$$\text{num} = \int_0^{k_F} \int_{-\pi/2}^{+\pi/2} k dk d\theta \frac{\hbar k}{m^*} \cos\theta = \frac{\hbar}{m^*} \int_0^{k_F} k^2 dk \int_{-\pi/2}^{+\pi/2} \cos\theta d\theta = \frac{\hbar}{m^*} \left(\frac{k_F^3}{3} \right) \times 2$$

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

$$\text{denom} = \int_0^{\infty} \int_{-\pi/2}^{+\pi/2} k dk d\theta f_0 = \int_0^{k_F} \int_{-\pi/2}^{+\pi/2} k dk d\theta = \int_0^{k_F} k dk \int_{-\pi/2}^{+\pi/2} d\theta = \frac{k_F^2}{2} \times \pi \quad (**)$$

Using (*) and (**)

$$\langle v_x^+ \rangle = \frac{\text{num}}{\text{denom}} = \frac{\left(\frac{2}{3} \right) \left(\frac{\hbar k_F^3}{m^*} \right)}{\pi k_F^2 / 2} = \frac{4}{3\pi} \frac{\hbar k_F}{m^*} = \frac{4}{3\pi} v_F$$

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$$\boxed{\langle v_x^+ \rangle = \frac{4}{3\pi} v_F}$$

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

3b) graphene

$$\langle v_x^+ \rangle = \frac{\sum_{k_x > 0, k_y} v_x(\vec{k}) f_0(E)}{\sum_{k_x > 0, k_y} f_0(E)} = \frac{\int_0^{\infty} \int_{-\pi/2}^{+\pi/2} k dk d\theta v_x f_0}{\int_0^{\infty} \int_{-\pi/2}^{+\pi/2} k dk d\theta f_0} = \frac{\text{num}}{\text{den}}$$

$$\text{num} = \int_0^{\infty} \int_{-\pi/2}^{+\pi/2} k dk d\theta v_x f_0 = \int_0^{\infty} \int_{-\pi/2}^{+\pi/2} k dk d\theta v_F \cos\theta f_0$$

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

$$\text{num} = \int_0^{k_F} \int_{-\pi/2}^{+\pi/2} k dk d\theta v_F \cos\theta = v_F \int_0^{k_F} k dk \int_{-\pi/2}^{+\pi/2} \cos\theta d\theta = v_F \left(\frac{k_F^2}{2} \right) \times 2$$

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

$$\text{den} = \int_0^{\infty} \int_{-\pi/2}^{+\pi/2} k dk d\theta f_0 = \int_0^{k_F} \int_{-\pi/2}^{+\pi/2} k dk d\theta = \int_0^{k_F} k dk \int_{-\pi/2}^{+\pi/2} d\theta = \frac{k_F^2}{2} \times \pi \quad (**)$$

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

$$\langle v_x^+ \rangle = \frac{\text{num}}{\text{den}} = \frac{v_F k_F^2}{k_F^2 \pi / 2} = \frac{2}{\pi} v_F$$

$$\boxed{\langle v_x^+ \rangle = \frac{2}{\pi} v_F}$$

ECE 656 Homework 2: (Week 2) (continued)

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

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

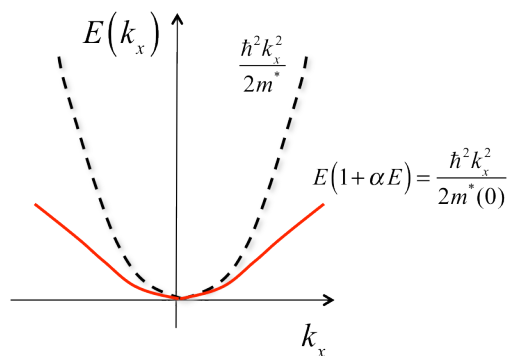
where

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

- 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.



- 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)

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

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

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

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

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

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.

ECE 656 Homework 2 (Week 2) (continued)**Solution:**

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

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

Note that $N(k)dk_x dk_y$ is the **number** of states per unit area. Now map these states onto energy:

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

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

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

The bandstructure is:

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

Differentiate with respect to k :

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

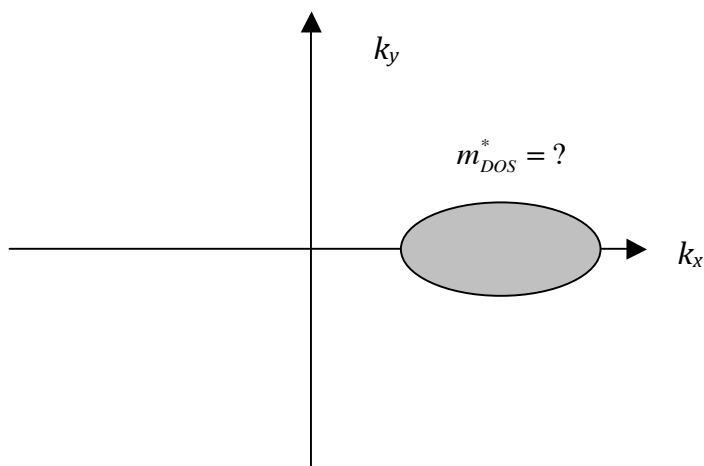
$$k \frac{dk}{dE} = \frac{m^*(0)}{\hbar^2} (1 + 2\alpha E) \quad (**)$$

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

$$\boxed{D_{2D}(E) = \frac{m^*(0)}{\pi \hbar^2} (1 + 2\alpha E)}$$

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.

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

Now define a “stretched” k-space:

$$\tilde{k}_x = \sqrt{\frac{m_0}{m_{xx}^*}} k_x \quad \tilde{k}_y = \sqrt{\frac{m_0}{m_{yy}^*}} k_y$$

ECE 656 Homework 2 (Week 2) (continued)

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

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

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

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

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

or, solving for the DOS:

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

Now use (*) to find:

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

and insert this in (**) to find

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

For the primed valleys of Si, $m_{xx}^* = m_\ell^*$ is the longitudinal effective mass and $m_{yy}^* = m_t^*$ 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

$$D'_{2D}(E) = g_v \frac{\sqrt{m_{xx} m_{yy}}}{\pi \hbar^2} = 4 \frac{\sqrt{m_\ell^* m_t^*}}{\pi \hbar^2},$$

ECE 656 Homework 2 (Week 2) (continued)

which can be written as

$$\boxed{D'_{2D}(E) = \frac{m_D^*}{\pi \hbar^2}$$

$$m_D^* = 4\sqrt{m_\ell^* m_t^*}}$$

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.

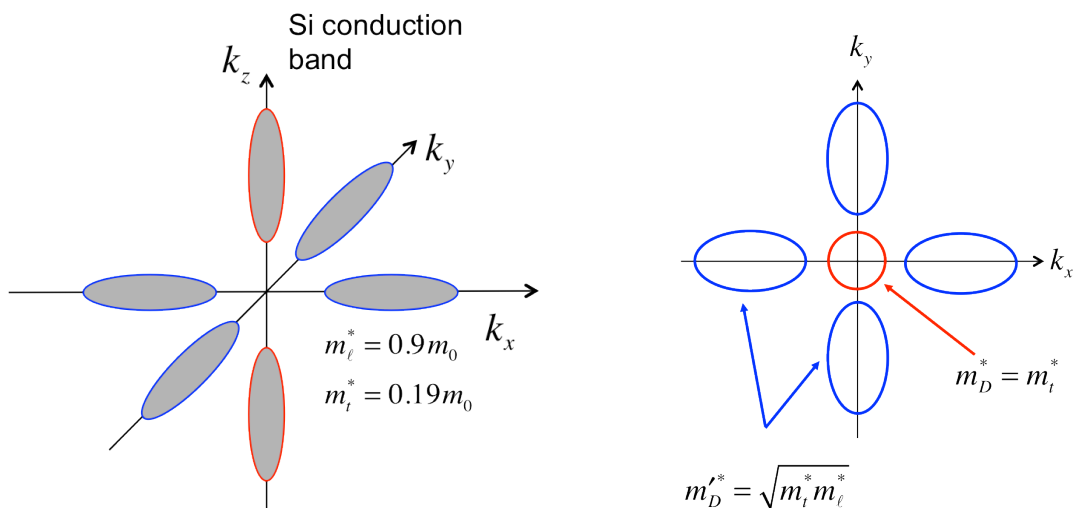
Unprimed valleys:

$$\epsilon_n = \frac{\hbar^2 n^2 \pi^2}{2m_\ell^2 t_{Si}^2} \quad D_{2D} = g_v \frac{m_t^*}{\pi \hbar^2} \quad g_v = 2$$

Primed valleys:

$$\epsilon'_n = \frac{\hbar^2 m^2 \pi^2}{2m_t^2 t_{Si}^2} \quad D'_{2D} = g'_v \frac{\sqrt{m_t^* m_\ell^*}}{\pi \hbar^2} \quad g'_v = 4$$

See the figures below:

ECE 656 Homework 2 (Week 2) (continued)**specific numbers: unprimed valleys:**

$$\varepsilon_n = \frac{\hbar^2 n^2 \pi^2}{2m_\ell^2 t_{Si}^2} = \frac{(0.042)}{m_\ell^*/m_0} n^2 \quad (\text{eV})$$

$$\varepsilon_1 = 0.046 \quad \varepsilon_2 = 0.185 \quad \varepsilon_3 = 0.415 \quad \varepsilon_4 = 0.739$$

$$D_{2D} = g_v \frac{m_t^*}{\pi \hbar^2} = 0.38 \frac{m_0}{\pi \hbar^2}$$

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

specific numbers primed valleys:

$$\varepsilon'_m = \frac{\hbar^2 m^2 \pi^2}{2m_t^2 t_{Si}^2} = \frac{(0.042)}{m_t^*/m_0} m^2 \quad (\text{eV})$$

$$\varepsilon'_1 = 0.221 \quad \varepsilon'_2 = 0.884 \quad \varepsilon'_3 = 1.989 \quad \varepsilon'_4 = 3.54$$

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

$$D_{2D} = g_v \frac{\sqrt{m_t^* m_\ell^*}}{\pi \hbar^2} = 1.66 \frac{m_0}{\pi \hbar^2}$$

ECE 656 Homework 2 (Week 2) (continued)

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

