SOLUTIONS: ECE 656 Homework 2 (Week 2)
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1)   Assume T = 0K 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.) (Assume a valley degeneracy of 2.)

   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:

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

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

$$n_S = \int_{E_C}^{E_F} g_V \frac{m^*}{\pi\hbar^2} dE = 2\frac{m^*}{\pi\hbar^2}(E_F - E_C)$$

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

     Case ii): graphene: DOS:

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

   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!

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

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

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

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

Case i): parabolic energy bands: DOS:

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

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

$$n_S = \frac{2m^*}{\pi\hbar^2}(E_F - E_C) \rightarrow n_S = \frac{2m^*}{\pi\hbar^2} \times \frac{\hbar^2 k_F^2}{2m^*} = g_V \times \frac{k_F^2}{2\pi}$$

$$\boxed{n_S = g_V \frac{k_F^2}{2\pi} = \frac{k_F^2}{\pi}}$$

Case ii): graphene: DOS:

$$E = \hbar v_F k \quad (E > 0)$$
$$E_F = \hbar v_F k_F \quad (E_F > 0)$$
$$n_S = \frac{E_F^2}{\pi\hbar^2 v_F^2} \rightarrow \frac{(\hbar v_F k_F)^2}{\pi\hbar^2 v_F^2} = \frac{k_F^2}{\pi}$$

$$\boxed{n_S = \frac{k_F^2}{\pi}} \qquad \text{(same as for parabolic energy bands)}$$

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 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

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

Working in k-space, we get the same answer for the two different band structures, because the DOS in k-space does not depend on band structure.

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.

   Your answers to these questions should be in terms of material parameters and the Fermi level.

Solution:

   2a) parabolic energy bands

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

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

   define:

$$\eta_F = \frac{E_F - E_C}{k_BT} \qquad \eta = \frac{E - E_C}{k_BT} \qquad d\eta = \frac{dE}{k_BT} \qquad dE = k_BT d\eta$$

   with this change of variables, we find:

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

   the integral can be done analytically:

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

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

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

so the answer is:

$$\boxed{\begin{aligned} n_S &= N_{2D}\mathcal{F}_0\left(\eta_F\right) \\ N_{2D} &= g_v \frac{m^* k_B T}{\pi\hbar^2} \end{aligned}}$$

2b) graphene

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

define:

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

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

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

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

$$\boxed{\begin{aligned} n_S &= N_{2D}\mathcal{F}_1\left(\eta_F\right) \\ N_{2D} &= \frac{2}{\pi}\left(\frac{k_B T}{\hbar v_F}\right)^2 \end{aligned}}$$

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

3)   Assume T = 0K 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

$$\left\langle v_x^+ \right\rangle = \frac{\sum\limits_{k_x>0,k_y} v_x\left(\vec{k}\right) f_0\left(E\right)}{\sum\limits_{k_x>0,k_y} f_0\left(E\right)} = \frac{\int\limits_0^\infty \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,v_x f_0}{\int\limits_0^\infty \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,f_0} = \frac{\text{num}}{\text{den}}$$ (DOS in k-space cancels from num

   and denom)

$$\text{num} = \int\limits_0^\infty \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,v_x f_0 = \int\limits_0^\infty \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,\frac{\hbar k}{m^*}\cos\theta\,f_0$$

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

$$\text{num} = \int\limits_0^{k_F} \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,\frac{\hbar k}{m^*}\cos\theta = \frac{\hbar}{m^*}\int\limits_0^{k_F} k^2\,dk \int\limits_{-\pi/2}^{+\pi/2}\cos\theta\,d\theta = \frac{\hbar}{m^*}\left(\frac{k_F^3}{3}\right)\times 2$$

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

$$\text{denom} = \int\limits_0^\infty \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,f_0 = \int\limits_0^{k_F} \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta = \int\limits_0^{k_F} k\,dk \int\limits_{-\pi/2}^{+\pi/2} d\theta = \frac{k_F^2}{2}\times\pi \qquad (**)$$

   Using (*) and (**)

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

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

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

3b) graphene

$$\left\langle v_x^+ \right\rangle = \frac{\sum\limits_{k_x>0,k_y} v_x(\vec{k})f_0(E)}{\sum\limits_{k_x>0,k_y} f_0(E)} = \frac{\int\limits_0^\infty \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,v_x f_0}{\int\limits_0^\infty \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,f_0} = \frac{\text{num}}{\text{den}}$$

$$\text{num} = \int\limits_0^\infty \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,v_x f_0 = \int\limits_0^\infty \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,v_F \cos\theta f_0$$

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

$$\text{num} = \int\limits_0^{k_F} \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,v_F \cos\theta = v_F \int\limits_0^{k_F} k\,dk \int\limits_{-\pi/2}^{+\pi/2} \cos\theta\,d\theta = v_F \left(\frac{k_F^2}{2}\right) \times 2$$

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

$$\text{den} = \int\limits_0^\infty \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta\,f_0 = \int\limits_0^{k_F} \int\limits_{-\pi/2}^{+\pi/2} k\,dk\,d\theta = \int\limits_0^{k_F} k\,dk \int\limits_{-\pi/2}^{+\pi/2} d\theta = \frac{k_F^2}{2} \times \pi \qquad (**)$$

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

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

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

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

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

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

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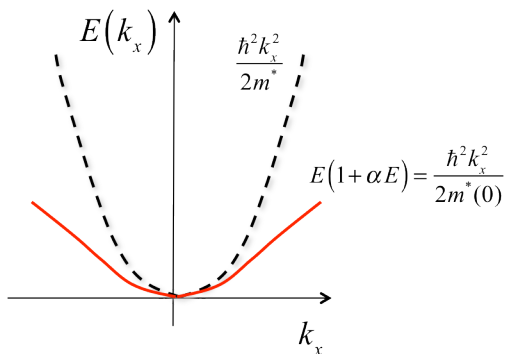
4b)   For this bandstructure, derive an expression for the velocity, $\upsilon_x(k_x)$ as a function of k_x.

Solution:
Velocity is related to bandstructure by:

$$\upsilon_x=\frac{1}{\hbar}\frac{dE}{dk_x}$$

ECE 656 Homework 2 (Week 2) (continued)

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

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

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

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

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

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

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

and write the velocity as

$$\upsilon_x = \frac{\hbar k_x}{m^*(E)}$$

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

$$D_{2D}(E) = g_v \frac{m^*}{\pi \hbar^2}\Theta(E - \varepsilon_1) \ .$$

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

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

and derive the density of states.

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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:

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

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

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

The bandstructure is:

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

Differentiate with respect to k:

$$\frac{d(E + \alpha E^2)}{dk} = \frac{dE}{dk}(1 + 2\alpha E)$$

from which we find

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

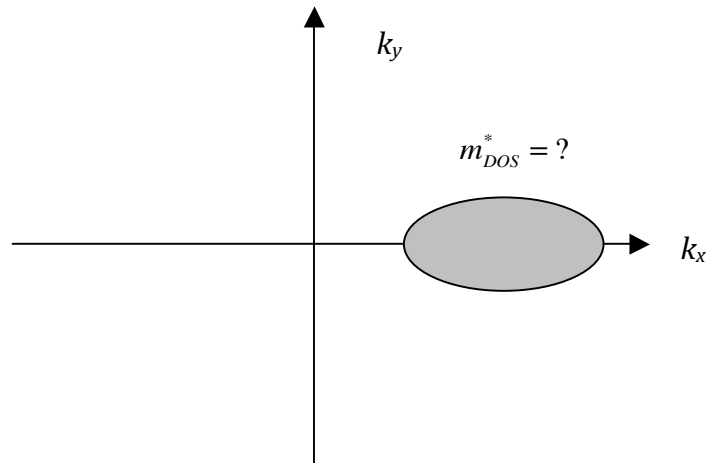$$k \frac{dk}{dE} = \frac{m^*(0)}{\hbar^2}(1 + 2\alpha E) \qquad\qquad (**)$$

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

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

So the 2D DOS increases linearly with energy when we take conduction band non-parabolicity into account.

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.

$$m^*_{DOS} = ?$$

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

Solution:

In this case, we write $E\left(k_x, k_y\right)$ 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 $E = \dfrac{\hbar^2 k_x^2}{2m^*_{xx}} + \dfrac{\hbar^2 k_y^2}{2m^*_{yy}}$ as $E = \dfrac{\hbar^2}{2m_0}\left[\left(\sqrt{\dfrac{m_0}{m^*_{xx}}}k_x\right)^2 + \left(\sqrt{\dfrac{m_0}{m^*_{yy}}}k_y\right)^2\right]$

Now define a "stretched" k-space:

$$\tilde{k}_x = \sqrt{\frac{m_0}{m^*_{xx}}}k_x \qquad\qquad \tilde{k}_y = \sqrt{\frac{m_0}{m^*_{yy}}}k_y$$

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

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

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

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

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

or, solving for the DOS:

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

Now use (*) to find:

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

and insert this in (**) to find

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

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

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

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which can be written as

$$\boxed{\begin{aligned} D'_{2D}(E) &= \frac{m_D^*}{\pi\hbar^2} \\ m_D^* &= 4\sqrt{m_\ell^* m_t^*} \end{aligned}}$$

The quantity, m_D^* is called the "density-of-states effective mass" (note that it includes the valley degeneracy the way we have defined it).

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.
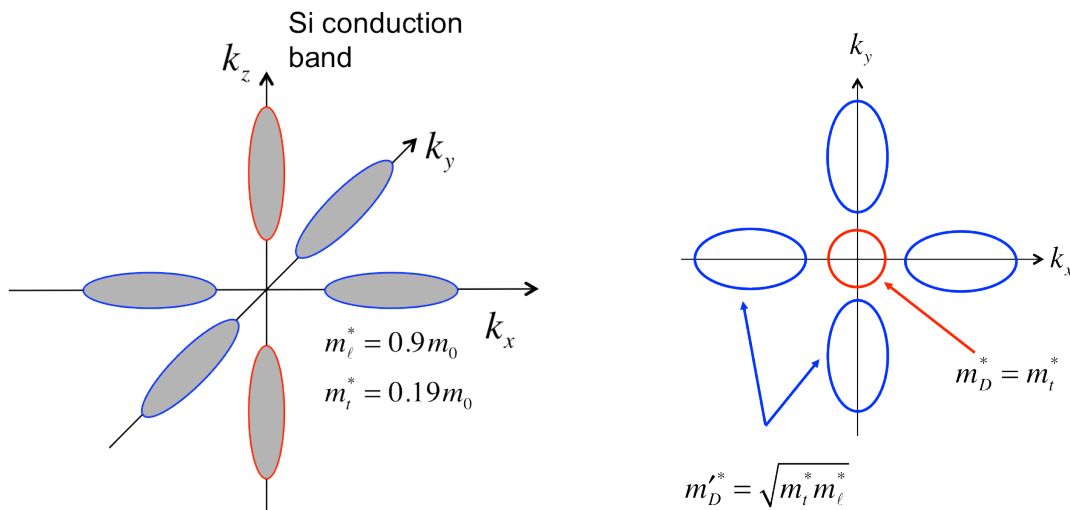
Unprimed valleys:

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

Primed valleys:

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

See the figures below:

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specific numbers: unprimed valleys:

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

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

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

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

specific numbers primed valleys:

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

$$\varepsilon_1' = 0.221 \qquad \varepsilon_2' = 0.884 \qquad \varepsilon_3' = 1.989 \qquad \varepsilon_4' = 3.54$$

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

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

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