ECE215A/MAT206A
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HW#7 Solutions

1. **Chapter 6, #2.**

(a). The wavevector at the corner is longer than the wavevector at the midpoint of a side by the factor $\sqrt{2}$. Since $U \propto k^2$ for a free electron, the energy is higher by $\left(\sqrt{2}\right)^2 = 2$.

(b). In 3D the energy is higher at a corner by $\left(\sqrt{3}\right)^2$ than at midpoint of a face.

(c). If the band gap at the midpoint of a face is less than the kinetic energy difference between this point and a corner, the electrons will spill-over into the n = 2 band in preference to filling the corner states in the n = 1 band. Divalent elements under these conditions will be metals and not insulators.

2. Chapter 6, #3

(a). We start with the "aliased" energy expression for the free electron, $U = \dfrac{\hbar^2 |\vec{k}+\vec{G}|^2}{2m}$,.

For k along the [111] direction, we can write from Kittel Chap. 2, $|\vec{k}| = \left(\dfrac{2\pi}{a}\right)(1,1,1)u$,

with $0 < u < \frac{1}{2}$, to stay within the 1st BZ below the Nyquist wave vector. The reciprocal lattice vectors can be written as

$\vec{G} = \left(\dfrac{2\pi}{a}\right)\left[(h-k+l)\hat{x} + (h+k-l)\hat{y} + (-h+k+l)\hat{z}\right]$, where h, k, l are any integers.

Thus $U = \left(\dfrac{\hbar^2}{2m}\right)\left(\dfrac{2\pi}{a}\right)^2 \left[(u+h-k+l)^2 + (u+h+k-l)^2 + (u-h+k+l)^2\right]$.

We now have to consider all combinations of indices h, k, l for which the term in brackets is smaller than $6\left[3(1/2)^2\right]$ = 9/2. This is done easily in Excel by trying all different permutations up to, say, h = k = l = 3, and then sorting. There are 15 resulting G vectors, specified by the Miller convention as G = (000); $(-1,-1,-1)$; $(-1,0,0)$, $(0,-1,0)$, and $(0,0,-1)$; (1,0,0), (0,1,0), and (0,0,1); (1,1,1); $(-1,-1,0)$, $(-1,0,-1)$, and $(0,-1,-1)$, (110), (101), and (011).

3. Chapter 6, #5

(a) Density of states of single ellipsoid

For ellipsoidal constant energy surface oriented along *x* axis we have

$$U\text{-}U_C = \frac{\hbar^2}{2}\left[\frac{(k_X - k_{X0})^2}{m_l} + \frac{(k_Y - k_{Y0})^2}{m_t} + \frac{(k_Z - k_{Z0})^2}{m_t}\right] \qquad (*)$$

From geometry we know that an ellipsoid $\frac{x^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2}=1$ has a volume given by V = (4/3)πabc. This makes us rewrite (*) as

$$1=\frac{\left(k_X-k_{X0}\right)^2}{2m_l\left(\Delta U\right)/\hbar^2}+\frac{\left(k_Y-k_{Y0}\right)^2}{2m_t\left(\Delta U\right)/\hbar^2}+\frac{\left(k_Z-k_{Z0}\right)^2}{2m_t\Delta U/\hbar^2}$$

where $\Delta U \equiv U-U_C$. So a constant energy U surface defined about $\vec{k}_0=\left(k_{X0},k_{Y0},k_{Z0}\right)$ will have a volume given by

$$V=\frac{4}{3}\pi\frac{\sqrt{2m_l\Delta U}}{\hbar}\frac{\sqrt{2m_t\Delta U}}{\hbar}\frac{\sqrt{2m_t\Delta U}}{\hbar}=\frac{4\pi}{3}\frac{\sqrt{m_lm_t^2}\left(2\Delta U\right)^{3/2}}{\hbar^3}$$

and $N\left(\vec{k}_0\right)\rightarrow N\left(U\right)=\frac{V}{4\pi^3}\frac{4\pi}{3}\frac{\sqrt{m_lm_t^2}\left(2\Delta U\right)^{3/2}}{\hbar^3}=\frac{V}{3\pi^2}\frac{\sqrt{m_lm_t^2}\left(2\Delta U\right)^{3/2}}{\hbar^3}$

$$g_n\left(U\right)=\frac{dN}{dU}=\frac{V}{3\pi^2}\frac{3}{2}\frac{2^{3/2}\sqrt{m_lm_t^2}\Delta U^{1/2}}{\hbar^3}=\frac{V\sqrt{2}\sqrt{m_lm_t^2}\left(U-U_C\right)^{1/2}}{\pi^2\hbar^3}.$$

If we define: $g\left(U\right)\equiv\frac{\sqrt{2}V\left(m_d^*\right)^{3/2}\left(U-U_c\right)}{\pi^2\hbar^3}$,

then $m_d^*=\left(m_lm_t^2\right)^{2/3}=\sqrt[3]{m_lm_t^2}$

and the specific density-of-states is

$$g'\left(U\right)=\frac{\sqrt{2}\sqrt{m_lm_t^2}\left(U-U_C\right)^{1/2}}{\pi^2\hbar^3}.$$

(b) Evaluation of key statistical mechanical properties for Si: At low temperature:
m_e=0.98 m_0, m_t=0.19 m_0, m_{lh}^*=0.16 m_0, m_{hh}^*=0.49 m_0, U_G=1.15 eV

a) so that density-of-states effective mass $\Rightarrow m_{d,c}^*=\sqrt[3]{m_em_t^2}=0.33\ m_0$

In valance band $m_d^* \Rightarrow m_{d,v}^*=\left[\left(m_{lh}^*\right)^{3/2}+\left(m_{hh}^*\right)^{3/2}\right]^{2/3}=0.55\ m_0$

These numbers are only valid at low temperatures. At 300 K, data tables show $m_{d,c}^*\approx 0.36$ because band gap drops and masses rise with temperature. Also, $m_{d,v}^*\approx 0.81\ m_0$ because m_{lh}^* & m_{hh}^* both increase too.

b) effective density-of-states

$$N_C(T) = \frac{M}{4}\left(\frac{2m_{d,c}^{*}k_BT}{\pi\hbar^2}\right)^{3/2} = 3.21\times10^{25}\ m^3 = 3.22\times10^{19}\ cm^3 \quad @\ 300\text{ K}$$

$$N_V(T) = \frac{1}{4}\left(\frac{2m_{d,v}^{*}k_BT}{\pi\hbar^2}\right)^{3/2} = 1.83\times10^{25}\ m^3 = 1.83\times10^{19}\ cm^3 \quad @\ 300\text{ K}$$

$$n_i(T) = \left(N_CN_V\right)^{1/2} e^{-U_G/2k_BT} = 1.14\times10^{10}\,cm^3$$

for U_G = 1.11 eV @ 300 K

At 450 K, masses change again; so does U_G

$$m_{d,C}^{*} \to 0.375m_0,\quad m_{d,V}^{*} \to 0.873m_0,\quad U_G \simeq 1.07\ \text{eV}$$

$N_C(T) \to 6.35\text{x}10^{19}\ cm^{-3}$, $N_V(T) \to 3.76\text{x}10^{19}\ cm^{-3}$, $n_i(T) \to 4.96\text{x}10^{13}\ cm^{-3}$

4. Chapter 6, #6

In vacuum, we know the hydrogen atom yields a ground state energy

$$U_1 = \frac{-\mu e^4}{(4\pi\varepsilon_0)^2\, 2\hbar^2}$$

and a wave function $$\psi_1 = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

where $\mu = \dfrac{m_em_p}{m_e+m_p} \approx m_e$ is the reduced mass and a_0 is the Bohr radius.

a) In semiconductors we dress the mass $m_e \to m_e^*$ and $\varepsilon_0 \to \varepsilon_r\varepsilon_0$, so that

$$U_1 \simeq \frac{-m_e^*e^4}{(4\pi\varepsilon_r\varepsilon_0)^2\, 2\hbar^2}.$$

b) In vacuum $a_0 \simeq \dfrac{4\pi\varepsilon_0\hbar^2}{m_ee^2}$. In a semiconductor this must be dressed so that

$$a_0 \approx \frac{4\pi\varepsilon_r\varepsilon_0\hbar^2}{m_e^* e^2} .$$

c) If impurities are uniformly distributed, we imagine each wave function as defining a sphere of radius a_0. Then put each sphere in box of width $2a_0$ so volume of box

$$= (2a_0)^3 \Rightarrow density = \frac{1}{volume} = \frac{1}{(2a_0)^3}$$

or

$$n_I \approx \left(\frac{m_e^* e^2}{8\pi\varepsilon_r\varepsilon_0\hbar^2} \right)^3 .$$

d) For GaAs $\varepsilon_r = 13,\ m^* = 0.067 m_0$

$$U_1 = \frac{-m_e^* e^4}{(4\pi\varepsilon_r\varepsilon_0)^2 2\hbar^2} = -13.6 \frac{m^*/m_0}{(\varepsilon_r)^2} = -0.0054 \quad eV$$

$$a_0 = \frac{4\pi\varepsilon_r\varepsilon_0\hbar^2}{m_e^* e^2} = 1.029 \times 10^{-8}$$, m = 10.3 nm

$$n_I = \frac{1}{(2a_0)^3} = 1.15\times10^{23}\mathrm{m}^{-3} = 1.15\mathrm{x}10^{17}\mathrm{cm}^{-3}$$