Physics 231, 2011 Final Exam, Solutions

1, (a) $\vec{a_1} = a(1,0)$

$\vec{a_2} = \frac{a}{2}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$

Reciprocal lattice vectors $\vec{b_1}$, $\vec{b_2}$, satisfy $\vec{b_i}\cdot\vec{a_j} = 2\pi\delta_{ij}$

$\Rightarrow \vec{b_2} = c(0,1)$ where c is determined from.

$\vec{b_2}\cdot\vec{a_2} = 2\pi$ so $c\,a\frac{\sqrt{3}}{2} = 2\pi$, so $c = \frac{4\pi}{\sqrt{3}}$

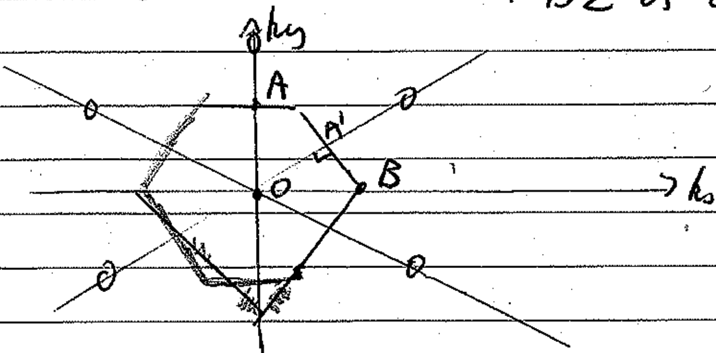
i.e. $\vec{b_2} = \frac{4\pi}{\sqrt{3}}\frac{1}{a}(0,1)$

$\vec{b_1} = c'(\sqrt{3},-1)$ and $\vec{b_1}\cdot\vec{a_1} = 2\pi$ which gives

$\vec{b_1} = \frac{4\pi}{\sqrt{3}}\frac{1}{a}\left(\frac{\sqrt{3}}{2}, \frac{-1}{2}\right)$

like $\vec{a_1}$ and $\vec{a_2}$, $\vec{b_1}$ and $\vec{b_2}$ make an angle of 60° with each other. Hence the reciprocal lattice is a triangular lattice

(b) Construct the Wigner-Seitz unit cell of the reciprocal lattice $\Rightarrow$ BZ is a hexagon.



$OA = \frac{1}{2}|\vec{b_1}| = \frac{2\pi}{\sqrt{3}}\frac{1}{a}$ Hence A is at $\frac{2\pi}{\sqrt{3}}\frac{1}{a}(0,1)$.

middle of an edge

$$OB = \frac{OA'}{\cos 30^\circ} = \frac{OA}{\cos 30^\circ} = \frac{2\pi}{\sqrt{3}} \frac{1}{a} \frac{2}{\sqrt{3}} = \frac{4\pi}{3} \frac{1}{a}$$

Hence B is at $\frac{4\pi}{3} \frac{1}{a} (1, 0)$ a corner of the BZ.

(c) Fourier transforming

$$\varepsilon(\vec{k}) = -t \sum_{\text{neighbors}} e^{i\vec{k}\cdot\vec{\delta}}$$ where $\vec{\delta}$ is the vector to a neighbor

$$= -t\left[2\cos k_x a + 4\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y \sqrt{3}\, a}{2}\right)\right]$$

(d)

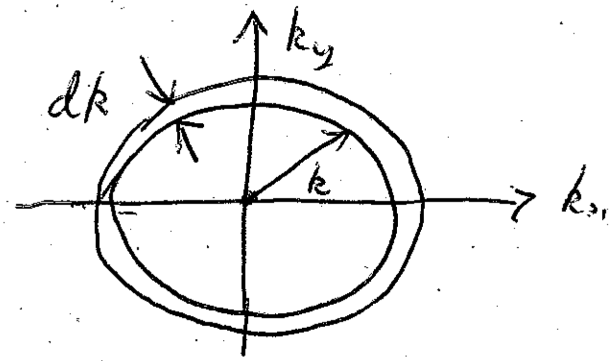
(i) At $\vec{k} = 0$, $\varepsilon(0) = -6t$

(ii) $\vec{k}$ at a corner is $\frac{4\pi}{3}\frac{1}{a}(1,0)$ ← (point B) from part (b) so

$$\varepsilon(\vec{k}_A) = -t\left[2\cos\frac{4\pi}{3} + 4\cos\frac{2\pi}{3}\right] = -t\left[2\left(-\tfrac{1}{2}\right) + 4\left(-\tfrac{1}{2}\right)\right] = +3t$$

(iii) $\vec{k}$ at the center of an edge (point A) is $\frac{2\pi}{\sqrt{3}}\frac{1}{a}(1,0)$

$$\Rightarrow \varepsilon(\vec{k}_B) = -t\left[2 + 4\cos\left(\frac{\sqrt{3}}{2}\frac{2\pi}{\sqrt{3}}\right)\right] = -t\left[2 + 4(-1)\right] = +2t$$



2 (a)

Number of ~~points~~ k-values inside a sphere of radius k is proportional to k^d

Hence number in the spherical shell shown $\propto k^{d-1}dk$

But $\omega = ck$ so

$$k^{d-1}dk \propto \omega^{d-1}d\omega$$

i.e. $\rho(\omega)d\omega \propto \omega^{d-1}d\omega$ so $\underline{\underline{\rho(\omega) \propto \omega^{d-1}}}$

(b) $$\frac{C}{k_B} = \int_0^\infty \rho(\omega)\left(\frac{\hbar\omega}{k_B T}\right)^2 \frac{e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega}-1\right)^2}\,d\omega \quad \text{(given)}$$

At low-T only the low-ω modes contribute so

$$C \propto \int_0^\infty \omega^{d-1}(\beta\hbar\omega)^2 \frac{e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega}-1\right)^2}\,d\omega$$

let $\beta\hbar\omega = x$ so

$$C \propto T^d \underbrace{\int_0^\infty \frac{x^{d+1}e^x}{(e^x-1)^2}\,dx}_{\text{a finite number}}$$

so $\underline{\underline{C \propto T^d}}$

3 (a) Density of points in k space is $\frac{A}{(2\pi)^2}$ so

$$2\times \frac{A}{(2\pi)^2} 2\pi k\,dk = g(\varepsilon)\,d\varepsilon$$

↑ spin

$$\Rightarrow d\varepsilon\, g(\varepsilon) = \frac{A}{\pi} k\,dk$$

Now $\varepsilon = \hbar v k$ so $k\,dk = \frac{1}{(\hbar v)^2} \varepsilon\, d\varepsilon$

$$\Rightarrow \underline{\underline{g(\varepsilon) = \frac{A}{\pi(\hbar v)^2}\varepsilon}}$$, i.e. linear density of states

(b) Fill states up to ε_F.

$$\Rightarrow N = \int_0^{\varepsilon_F} g(\varepsilon)\,d\varepsilon = \frac{A}{\pi(\hbar v)^2}\frac{\varepsilon_F^2}{2}$$

so $\underline{\underline{\varepsilon_F = (2\pi n)^{1/2}\hbar v}}$ where $n \equiv \frac{N}{A}$ is the number per unit area.

(c) Ground state energy is given by

$$E = \int_0^{\varepsilon_F} \varepsilon\, g(\varepsilon)\,d\varepsilon = \frac{A}{\pi(\hbar v)^2}\frac{\varepsilon_F^3}{3}$$

$$= \underbrace{\frac{A}{\pi(\hbar v)^2}\frac{\varepsilon_F^2}{2}}_{N}\varepsilon_F \frac{2}{3}$$

$$= \frac{2}{3}N\varepsilon_F \quad \text{so} \quad \underline{\underline{\frac{E}{N} = \frac{2}{3}\varepsilon_F}}$$

4/ (a) ε_c

--- μ

ε_v

$$f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$$

Now for ε in the conduction band $\varepsilon-\mu \gg k_BT$ so $f(\varepsilon) \simeq e^{-\beta(\varepsilon-\mu)}$

For ε in the valence band, $\mu-\varepsilon \gg k_BT$ so that

$$\underbrace{1-f(\varepsilon)}_{\text{hole occupancy}} = \cancel{e^{\beta(\varepsilon-\mu)}+1} \quad \frac{1}{e^{-\beta(\varepsilon-\mu)}+1} \simeq e^{-\beta(\mu-\varepsilon)}.$$

Hence $n_c(T) = \int_{\varepsilon_c}^{\infty} g_c(\varepsilon)\, e^{-\beta(\varepsilon-\mu)}\, d\varepsilon$ $\qquad (x = \varepsilon-\varepsilon_c)$

$$= \frac{\sqrt{2}\, m_c^{3/2}}{\hbar^3\pi^2}\, e^{-\beta(\varepsilon_c-\mu)} \underbrace{\int_0^{\infty} e^{-\beta x} x^{1/2}\, dx}_{(k_BT)^{3/2}\underbrace{\int_0^{\infty} y^{1/2} e^{-y}\, dy}_{\frac{1}{2}\sqrt{\pi}}} \qquad x\beta = y$$

$$= \underbrace{\frac{1}{4}\left(\frac{2m_c k_BT}{\pi\hbar^2}\right)^{3/2}}_{N_c(T)} e^{-\beta(\varepsilon_c-\mu)}$$

Similarly $p_v(T) = \int_{-\infty}^{\varepsilon_v} g_v(\varepsilon)\,[1-f(\varepsilon)]$

which gives $p_v(T) = P_v(T)\, e^{-\beta(\mu-\varepsilon_v)}$

where $P_v(T) = \frac{1}{4}\left(\frac{2m_v k_BT}{\pi\hbar^2}\right)^{3/2}$

(b) Impurities levels alter the value for μ but these expressions, expressed in terms of μ are valid whether or not there are impurity levels because they only depend on the density of states in the band and the Fermi function

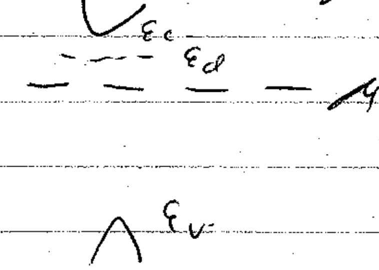
(c) If there are no impurities, $n_c = p_v$ so

$$n_c = p_v = \sqrt{n_c p_v}$$

↑ independent of μ.

$$= \left(N_c(T)\,P_v(T)\right)^{1/2} e^{-(\varepsilon_c - \varepsilon_v)/2k_BT} \quad (= n_i \text{ say})$$

(d) If there are donor impurities these are easily excited into the conduction band.
Hence μ is ~~raised~~ to be close to the ~~do~~ energy of the donor levels



n_c is increased ~~to be~~ since ~~electrons are~~ electrons are easily excited into the conduction band from the donor levels

However, from part (a) $n_c p_v = n_i^2$ is independent of impurities.

Hence $p_v = \dfrac{n_i^2}{n_c}$ must decrease (since n_c increases).