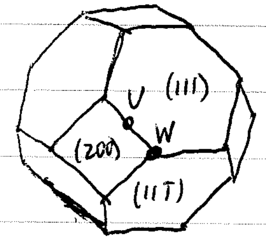
PHY 521 Solutions Problem Set 6

1) a) pt W in k-space lies at the intersection of 3 Bragg planes that bisect the R.L. vectors



$$\vec{K}_1 = \frac{2\pi}{a}(1,1,1)$$
$$\vec{K}_2 = \frac{2\pi}{a}(1,1,-1)$$
$$\vec{K}_3 = \frac{2\pi}{a}(2,0,0)$$

Pt W is at $\vec{k}_W = \frac{2\pi}{a}(1,\frac{1}{2},0)$

In the weak potential approximation, for $\vec{k}$ near $\vec{k}_W$ we need to consider scattering off all three Bragg planes. The matrix equation to solve is

$$(\varepsilon^0_{k-K_i} - \varepsilon)\, c_{k-K_i} + \sum_j U_{K_j-K_i}\, c_{k-K_j} = 0$$

where the only K_i's that enter are $\{0, \vec{K}_1, \vec{K}_2, \vec{K}_3\}$

One then gets a 4x4 matrix equation:

$$\begin{pmatrix} \varepsilon^0_k - \varepsilon & U_{K_1} & U_{K_2} & U_{K_3} \\ U_{-K_1} & \varepsilon^0_{k-K_1} - \varepsilon & U_{K_2-K_1} & U_{K_3-K_1} \\ U_{-K_2} & U_{K_1-K_2} & \varepsilon^0_{k-K_2} - \varepsilon & U_{K_3-K_2} \\ U_{-K_3} & U_{K_1-K_3} & U_{K_2-K_3} & \varepsilon^0_{k-K_3} - \varepsilon \end{pmatrix} \begin{pmatrix} c_k \\ c_{k-K_1} \\ c_{k-K_2} \\ c_{k-K_3} \end{pmatrix} = 0$$

By cubic symmetry of the crystal, $U_{K_1} = U_{K_2} \equiv U_1$

By inversion symmetry $U_{-K_1} = U_{K_1}$ and $U_{-K_2} = U_{K_2}$

so $U_{K_1} = U_{K_2} = U_{-K_1} = U_{-K_2} \equiv U_1$

Also, $\vec{K}_1 - \vec{K}_3 = \frac{2\pi}{a}(-1,1,1)$ and $\vec{K}_2 - \vec{K}_3 = \frac{2\pi}{a}(-1,1,-1)$

so by cubic symmetry and inversion symmetry

$$U_{K_1-K_3} = U_{K_3-K_1} = U_{K_2-K_3} = U_{K_3-K_2} = U_1$$

Also, $\vec{K}_1 - \vec{K}_2 = \frac{2\pi}{a}(0,0,2)$.

so by cubic and inversion symmetries

$$U_{K_1-K_2} = U_{K_2-K_1} = U_{K_3} = U_{-K_3} \equiv U_2$$

So matrix equation becomes

$$\begin{pmatrix} \varepsilon_k^0 - \varepsilon & U_1 & U_1 & U_2 \\ U_1 & \varepsilon_{k-K_1}^0 - \varepsilon & U_2 & U_1 \\ U_1 & U_2 & \varepsilon_{k-K_2}^0 - \varepsilon & U_1 \\ U_2 & U_1 & U_1 & \varepsilon_{k-K_3}^0 - \varepsilon \end{pmatrix} \begin{pmatrix} c_k \\ c_{k-K_1} \\ c_{k-K_2} \\ c_{k-K_3} \end{pmatrix} = 0$$

Finally, exactly at $\vec{k} = \vec{k}_W$, the states $\vec{k}_W$, $\vec{k}_W - \vec{K}_1$, $\vec{k}_W - \vec{K}_2$, $\vec{k}_W - \vec{K}_3$ are degenerate, so

$$\varepsilon_k^0 = \varepsilon_{k-K_1}^0 = \varepsilon_{k-K_2}^0 = \varepsilon_{k-K_3}^0 \equiv \varepsilon_W^0 = \frac{\hbar^2 k_W^2}{2m}$$

and the matrix equation becomes

$$\begin{pmatrix} \varepsilon_W^0 - \varepsilon & U_1 & U_1 & U_2 \\ U_1 & \varepsilon_W^0 - \varepsilon & U_2 & U_1 \\ U_1 & U_2 & \varepsilon_W^0 - \varepsilon & U_1 \\ U_2 & U_1 & U_1 & \varepsilon_W^0 - \varepsilon \end{pmatrix} \begin{pmatrix} c_{k_W} \\ c_{k_W-K_1} \\ c_{k_W-K_2} \\ c_{k_W-K_3} \end{pmatrix} = 0$$

For this system of homogeneous linear equations to have a non trivial solution, the determinant of the matrix must vanish

$$\begin{vmatrix} \varepsilon_W^0 - \varepsilon & U_1 & U_1 & U_2 \\ U_1 & \varepsilon_W^0 - \varepsilon & U_2 & U_1 \\ U_1 & U_2 & \varepsilon_W^0 - \varepsilon & U_1 \\ U_2 & U_1 & U_1 & \varepsilon_W^0 - \varepsilon \end{vmatrix} = 0$$

the solutions ε to the above are just the 4 eigenvalues of the matrix

$$\begin{pmatrix} \varepsilon_W^0 & U_1 & U_1 & U_2 \\ U_1 & \varepsilon_W^0 & U_2 & U_1 \\ U_1 & U_2 & \varepsilon_W^0 & U_1 \\ U_2 & U_1 & U_1 & \varepsilon_W^0 \end{pmatrix}$$

For such a symmetrix matrix, rather than solve the 4th order polynomial equation for the eigenvalues ε, it is easier just to <u>guess</u> the eigenvectors

$$\begin{pmatrix} \varepsilon_W^0 & U_1 & U_1 & U_2 \\ U_1 & \varepsilon_W^0 & U_2 & U_1 \\ U_1 & U_2 & \varepsilon_W^0 & U_1 \\ U_2 & U_1 & U_1 & \varepsilon_W^0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \varepsilon \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix}$$

$\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$ gives $\varepsilon = \varepsilon_W^0 + 2U_1 + U_2$

$\begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}$ gives $\varepsilon = \varepsilon_W^0 - U_2$

$\begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}$ gives $\varepsilon = \varepsilon_W^0 - U_2$

$\begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}$ gives $\varepsilon = \varepsilon_W^0 - 2U_1 + U_2$

so we get energies $\varepsilon_W^0 + 2U_1 + U_2$, $\varepsilon_W^0 - 2U_1 + U_2$, $\varepsilon_W^0 - U_2$ (doubly degenerate)

b) For $\vec{k}$ near $\vec{k}_U = \frac{2\pi}{a}(1, \frac{1}{4}, \frac{1}{4})$, we need to consider scattering off only the two Bragg planes that bisect the R.L. vectors $\vec{K}_1$ and $\vec{K}_3$. The resulting 3×3 matrix equation to solve is

$$\begin{pmatrix} \varepsilon_k^0 - \varepsilon & U_{K_1} & U_{K_3} \\ U_{-K_1} & \varepsilon_{k-K_1}^0 - \varepsilon & U_{K_3-K_1} \\ U_{-K_3} & U_{K_1-K_3} & \varepsilon_{k-K_3}^0 - \varepsilon \end{pmatrix} \begin{pmatrix} c_k \\ c_{k-K_1} \\ c_{k-K_3} \end{pmatrix} = 0$$

Using $U_{K_1} = U_{-K_1} = U_{K_1-K_3} = U_{K_3-K_1} \equiv U_1$

and $U_{K_3} = U_{-K_3} \equiv U_2$

And at $\vec{k} = \vec{k}_U$, $\varepsilon_{k_U}^0 = \varepsilon_{k_U-K_1}^0 = \varepsilon_{k_U-K_3}^0 \equiv \varepsilon_U^0 = \frac{\hbar^2 k_U^2}{2m}$

we get

$$\begin{pmatrix} \varepsilon_U^0 - \varepsilon & U_1 & U_2 \\ U_1 & \varepsilon_U^0 - \varepsilon & U_1 \\ U_2 & U_1 & \varepsilon_U^0 - \varepsilon \end{pmatrix} \begin{pmatrix} c_{k_U} \\ c_{k_U-K_1} \\ c_{k_U-K_3} \end{pmatrix} = 0$$

or $$\begin{pmatrix} \varepsilon_U^0 & U_1 & U_2 \\ U_1 & \varepsilon_U^0 & U_1 \\ U_2 & U_1 & \varepsilon_U^0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \varepsilon \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

We can guess one eigenvector

$\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$ gives $\varepsilon = \varepsilon_U^0 - U_2$

It is harder to guess the other two eigenvectors.
~~Instead of trying to guess, we can project the~~

Instead, lets solve the characteristic equation for the eigenvalues ε. Let $\delta\varepsilon \equiv \varepsilon_U^0 - \varepsilon$. Then we have

$$\det \begin{pmatrix} \delta\varepsilon & U_1 & U_2 \\ U_1 & \delta\varepsilon & U_1 \\ U_2 & U_1 & \delta\varepsilon \end{pmatrix} = 0$$

$$\Rightarrow \quad \delta\varepsilon\left[\delta\varepsilon^2 - U_1^2\right] - U_1\left[U_1\delta\varepsilon - U_1U_2\right] + U_2\left[U_1\delta\varepsilon - U_1U_2\right] = 0$$

$$\Rightarrow \delta\varepsilon^3 - (2U_1^2 + U_2^2)\,\delta\varepsilon + 2U_1^2U_2 = 0$$

We already know that from the eigenvector we guessed, one solution is $\delta\varepsilon = \varepsilon_U^0 - \varepsilon = U_2$. So factor off this root from the cubic polynomial

$$\delta\varepsilon^3 - (2U_1^2 + U_2^2)\delta\varepsilon + 2U_1^2U_2$$
$$= (\delta\varepsilon - U_2)(\delta\varepsilon^2 + a\,\delta\varepsilon + b)$$ expand to determine a and b

$$\Rightarrow a = U_2, \quad b = -2U_1^2$$

So we are now left with a quadratic equation for the two remaining unknown eigenvalues

$$\delta\varepsilon^2 + U_2\delta\varepsilon - 2U_1^2 = 0$$

$$\delta\varepsilon = -\frac{U_2}{2} \pm \sqrt{\frac{U_2^2}{4} + 2U_1^2} \qquad = \varepsilon_U^0 - \varepsilon$$

$$\varepsilon = \varepsilon_U^0 + \frac{U_2}{2} \pm \sqrt{\frac{U_2^2}{4} + 2U_1^2}$$

$$= \varepsilon_U^0 + \frac{U_2}{2} \pm \frac{1}{2}\sqrt{U_2^2 + 8U_1^2}$$

So finally the three energies at pt U are

$$\varepsilon_U^0 - U_2$$

$$\varepsilon_U^0 + \frac{U_2}{2} \pm \frac{1}{2}\sqrt{U_2^2 + 8U_1^2}$$

2) a) $\varepsilon(\vec{k}) = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right)$

constant energy surface of energy ε is therefore given by the ellipsoid equation

$$1 = \left(\frac{\hbar^2}{2\varepsilon m_x}\right)k_x^2 + \left(\frac{\hbar^2}{2\varepsilon m_y}\right)k_y^2 + \left(\frac{\hbar^2}{2\varepsilon m_z}\right)k_z^2$$

and so contains a volume of k-space equal to

$$v = \left(\frac{4\pi}{3}\right)\left[\left(\frac{2\varepsilon}{\hbar^2}\right)^3 m_x m_y m_z\right]^{1/2}$$

The volume of k-space per allowed k-vector is

$$(\Delta k)^3 = \frac{(2\pi)^3}{V}$$ where V is volume of the system

So the number of electron states with energy less than ε (ie those contained with the volume of the above ellipsoid) is

$$V\,G(\varepsilon) = \frac{\underset{\text{2 spin states for each } \vec{k}}{2} \cdot \frac{4\pi}{3}\left[\left(\frac{2\varepsilon}{\hbar^2}\right)^3 m_x m_y m_z\right]^{1/2}}{\left(\frac{(2\pi)^3}{V}\right)} = \frac{2v}{(\Delta k)^3}$$

So the number of electron states per volume with energy less than ε is

$$G(\varepsilon) = \frac{1}{3\pi^2\hbar^3}\, 2^{3/2}\, \varepsilon^{3/2}\, (m_x m_y m_z)^{1/2}$$

So the density of states is

$$g(\varepsilon) = \frac{dG}{d\varepsilon} = \frac{1}{3\pi^2\hbar^3}\,\frac{3}{2}\,2^{3/2}\,\varepsilon^{1/2}\,(m_x m_y m_z)^{1/2}$$

$$\boxed{g(\varepsilon) = \frac{1}{\pi^2\hbar^3}\sqrt{2(m_x m_y m_z)\,\varepsilon}}$$

Compare this to the free electron result, which we get by taking $m = m_x = m_y = m_z$

$$g_{free}(\varepsilon) = \frac{1}{\pi^2\hbar^3}\sqrt{2m^3\varepsilon}$$

$$= \frac{m}{\pi^2\hbar^2}\sqrt{\frac{2m\varepsilon}{\hbar^2}}$$ ← more familiar form from, say AM Eq (2.…

Comparing, we see that the anisotropic case looks just like the free electron provided we use an effective mass

$$\boxed{m^* = (m_x m_y m_z)^{1/3}}$$

b) Electronic specific heat $C_V = \gamma T$ at low T, where

$\gamma \propto g(\varepsilon_F)$ density of states at the Fermi energy

We need to ~~fig~~ find ε_F. For a fixed density n of conduction electrons

$$n = \int_0^{\varepsilon_F} g(\varepsilon)\,d\varepsilon = G(\varepsilon_F) = \frac{1}{3\pi^2\hbar^3}\,2^{3/2}\,\varepsilon_F^{3/2}\,m^{*\,3/2}$$

So $$\varepsilon_F = \left(\frac{3\pi^2\hbar^3 n}{2^{3/2} m^{*3/2}}\right)^{2/3} = \frac{(3\pi^2\hbar^3)^{2/3}}{2m^*}$$

So $\varepsilon_F \propto \frac{1}{m^*}$

Then $$g(\varepsilon_F) = \frac{1}{\pi^2\hbar^3}\sqrt{2m^{*3}\frac{(3\pi^2\hbar^3)^{2/3}}{2m^*}}$$

$$= \frac{(3\pi^2\hbar^3)^{1/3}}{\pi^2\hbar^3}\, m^* \quad \propto m^*$$

So $\boxed{\gamma \propto g(\varepsilon_F) \propto m^*}$