ECE 4070: Prelim Exam 2 Solutions

Problem 2

a) In the long wavelength limit (i.e. for $|\vec{q}| \approx 0$), all atoms in the crystal move in phase for the acoustic modes. This means that during the motion no bonds are stretched or bent (i.e. no springs are compressed or stretched or bent) and therefore the energy required to excite such modes becomes vanishingly small in the long wavelength limit. In case of the optical modes, the atoms in the same primitive cell move out of phase and therefore bonds within the same primitive cell are always stretched or bent during motion even in the long wavelength limit (i.e. for $|\vec{q}| \approx 0$). Therefore, there is an energy cost associated with exciting optical modes in the ling wavelength limit, and therefore $\hbar\omega(\vec{q}) \neq 0$ when $|\vec{q}| \rightarrow 0$.

b) Consider the dynamical equation, $\overline{\overline{D}}(\vec{q})\vec{u}(\vec{q}) = \omega(\vec{q})^2\overline{\overline{M}}\vec{u}(\vec{q})$. Suppose we have solved it. Now let $\vec{q} \rightarrow -\vec{q}$, we get, $\overline{\overline{D}}(-\vec{q})\vec{u}(-\vec{q}) = \omega(-\vec{q})^2\overline{\overline{M}}\vec{u}(-\vec{q}) \quad \Rightarrow \quad \overline{\overline{D}}^*(\vec{q})\vec{u}(-\vec{q}) = \omega(-\vec{q})^2\overline{\overline{M}}\vec{u}(-\vec{q})$

Now complex conjugate both sides, and realizing that frequencies are always real, one gets,

$\overline{\overline{D}}(\vec{q})\vec{u}^*(-\vec{q}) = \omega(-\vec{q})^2\overline{\overline{M}}\vec{u}^*(-\vec{q})$

Since one has now the same matrix $\overline{\overline{D}}(\vec{q})$ on the left hand side as in the original case, the frequencies will be the same as that in the original case, i.e. $\omega(-\vec{q}) = \omega(\vec{q})$. We also get the additional result, $\vec{u}(-\vec{q}) = \vec{u}^*(\vec{q})$. The result $\omega(-\vec{q}) = \omega(\vec{q})$ is a consequence of the time reversal symmetry of Newton's second law.

c) First consider the two pockets at the K-points: $\left(-\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{3a}\right)$ and at $\left(\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{3a}\right)$. The conductivity tensor $\overline{\overline{\sigma}}$ for both will be proportional to their respective $\overline{\overline{M}}^{-1}$. If one applies E-field in the +y-direction, then the current in the +y-direction ought to be the same for both by symmetry. This means $\overline{\overline{M}}_{yy}^{-1}$ is the same for both. Similarly, if one applies E-field in the x-direction then the current in the x-direction for $\left(\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{3a}\right)$ pocket ought to be the same as the current in the –x-direction for the pocket at $\left(-\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{3a}\right)$ under an E-field in the –x-direction. This means $\overline{\overline{M}}_{xx}^{-1}$ is also the same for both. Now if one applies an E-field in the +y-direction, and looks at the current in the x-direction, it should have opposite signs for the two pockets and this implies that the off-diagonal components of $\overline{\overline{M}}^{-1}$ have opposite signs for the two pockets. Therefore for the pocket at $\left(\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{3a}\right)$ we must have:

$$\overline{\overline{M}}^{-1} = \begin{bmatrix} 1/m_1 & -(1/m_2 - 1/m_1)\sqrt{3}/2 \\ -(1/m_2 - 1/m_1)\sqrt{3}/2 & 1/m_2 \end{bmatrix}$$

Now consider the pocket at $\left(0, \frac{4\pi}{3a}\right)$. If an E-field is applied in the +y-direction, there cannot be any net current in the x-direction (since both +x-direction and –x-direction are equivalent by symmetry and the current cannot choose to flow in one and not in the other direction). Therefore, $\overline{\overline{M}}^{-1}$ must be diagonal for this pocket. So all we need to do is to find a diagonalized version of the given $\overline{\overline{M}}^{-1}$ for the pocket at $\left(-\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{3a}\right)$ (i.e. find its eigenvalues) and the result is:

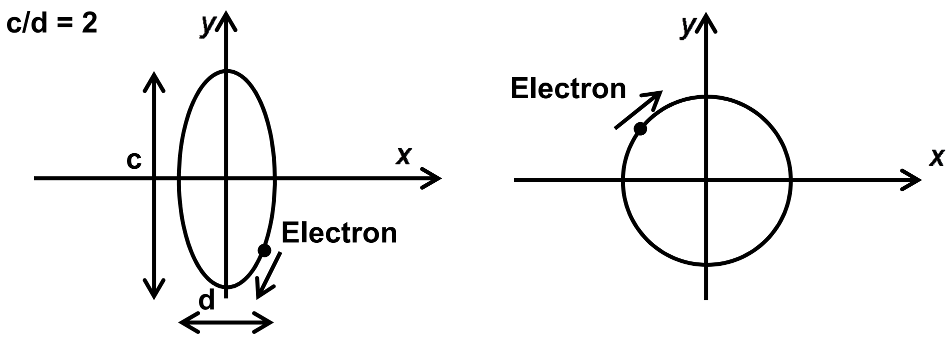
$$\overline{\overline{M}}^{-1} = \begin{bmatrix} 3/2m_2 - 1/2m_1 & 0 \\ 0 & 3/2m_1 - 1/2m_2 \end{bmatrix}$$

Problem 1

a) and b) Note that the group velocity in real space is always perpendicular to a constant energy surface in k-space. For a parabolic valence band, the velocity points inwards from the surface and outwards for a parabolic conduction band. One also has the relation from the homework problem:

$$\vec{r}_\perp(t) - \vec{r}_\perp(t=0) = -\frac{\hbar}{e|\vec{B}|^2}\vec{B} \times \left[\vec{k}(t) - \vec{k}(t=0)\right]$$

That tells that the trajectory in real space is a rotated version of the trajectory in k-space. With this information we can draw the trajectories as shown below (the real space origin is chosen arbitrarily).



c) From your homework, the electron cyclotron frequency for a B-field in a particular direction is given by the square-root of the determinant of the inverse effective sub-matrix in the other two dimensions. So for the B-field in the x, y, and z-directions, the cyclotron frequencies are: $eB_o/\sqrt{m_{yy}m_{zz}}$, $eB_o/\sqrt{m_{xx}m_{zz}}$, and $eB_o/\sqrt{m_{xx}m_{yy}}$, respectively. This gives: $m_{xx} = 0.1m_o$, $m_{yy} = 0.4m_o$, $m_{zz} = 0.9m_o$.

d) $E(\vec{k}) = E_c + ak^4 \quad \Rightarrow \vec{v}(\vec{k}) = 4\frac{a}{\hbar}k^3\hat{k} = 4\frac{a}{\hbar}(\vec{k}.\vec{k})\vec{k}$. The expression for the current is:

$$\vec{J} = -e \times 2 \times \int \frac{d^3\vec{k}}{(2\pi)^3}\; f\left(\vec{k} + \frac{e\tau\,\vec{E}}{\hbar}\right)\vec{v}(\vec{k})$$

$$= -2e \times \int \frac{d^3\vec{k}}{(2\pi)^3}\; f(\vec{q})\,\vec{v}\left(\vec{k} - \frac{e\tau\,\vec{E}}{\hbar}\right) = -2e \times \int \frac{d^3\vec{k}}{(2\pi)^3}\; f(\vec{k})\,4\frac{a}{\hbar}\left[\left(\vec{k} - \frac{e\tau\,\vec{E}}{\hbar}\right).\left(\vec{k} - \frac{e\tau\,\vec{E}}{\hbar}\right)\right]\left(\vec{k} - \frac{e\tau\,\vec{E}}{\hbar}\right)$$

$$= -8ae \times \int \frac{d^3\vec{k}}{(2\pi)^3}\; f(\vec{k})\left[k^2\,\vec{k} - \frac{2e\tau(\vec{k}.\vec{E})\vec{k}}{\hbar} - \frac{e\tau\,k^2\vec{E}}{\hbar} + \ldots\right] = 8\frac{a}{\hbar}e \times \int \frac{d^3\vec{k}}{(2\pi)^3}\; f(\vec{k})\left[\frac{5e\tau k^2}{3\hbar}\right]\vec{E}$$

Where only terms linear in the E-field have been retained and the equilibrium term has been ignored. The spherically symmetric integral over the k-space is elementary at near-zero temperature and the result is,

$$\vec{J} = \frac{4}{3}a\frac{e^2\tau\,k_F^5}{\pi^2\hbar^2} \times \vec{E} = \sigma\,\vec{E}$$

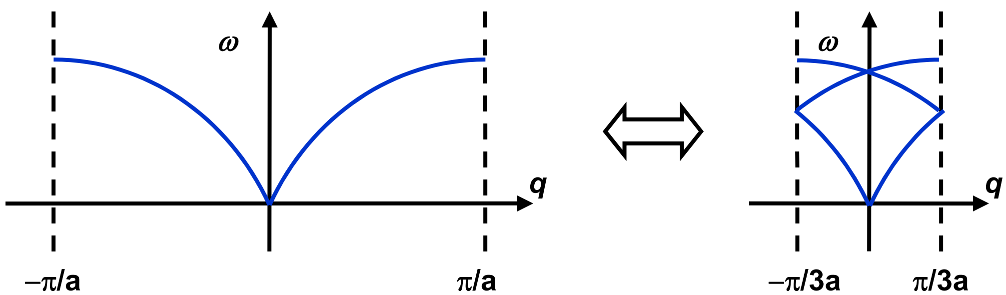
Problem 3

a) $$\begin{bmatrix} 2\alpha & -\alpha\, e^{iqa} & -\alpha\, e^{-iqa} \\ -\alpha\, e^{-iqa} & (\alpha+\beta) & -\beta\, e^{iqa} \\ -\alpha\, e^{iqa} & -\beta\, e^{-iqa} & (\alpha+\beta) \end{bmatrix} \begin{bmatrix} u_1(q) \\ u_2(q) \\ u_3(q) \end{bmatrix} = \omega^2 \begin{bmatrix} M_1 & & \\ & M_2 & \\ & & M_2 \end{bmatrix} \begin{bmatrix} u_1(q) \\ u_2(q) \\ u_3(q) \end{bmatrix}$$

Note that the size of the primitive cell is $3a$ and the size of the FBZ is $2\pi/3a$.

b) If $M_1 = M_2$ the lattice symmetry is not affected in any way since the spring constants still dictate that the primitive cell and the FBZ are of the same sizes as before. So one would not expect the bandgap to close.

c) If $M_1 = M_2$ and $\alpha = \beta$ then as far as the phonons are concerned the actual primitive cell is of size a and the FBZ is of size $2\pi/a$ and there is only one acoustic band. However, within the old FBZ of size $2\pi/3a$ one will observe three bands (one acoustic and two optical). These bands will be identical to the single acoustic band of the larger FBZ folded into the smaller FBZ. Therefore, the lowest two will be degenerate at the zone edges and the upper two bands will be degenerate at the zone center, as shown below.



d) The dispersion relation for a single acoustic band with spring constant α and lattice constant a is form the lecture notes equal to $\omega(q) = \sqrt{4\alpha/M_1}\,\sin(qa/2)$ (LEFT FIG). Therefore, the frequency of the two degenerate optical phonons bands at the zone center in the smaller FBZ (RIGHT FIG) is equal to $\omega(q) = \sqrt{4\alpha/M_1}\,\sin(qa/2)\Big|_{q=2\pi/3a} = \sqrt{3\alpha/M_1}$. Third frequency is zero (acoustic band at zone center).

You can check the result by direct solution of the matrix equation above.