ECE4070: Homework 8 Solutions

Problem 8.1

a)
$$\overline{\overline{D}}(\vec{q}) = \begin{bmatrix} 2\alpha[1-\cos(q_x a)\cos(q_y a)] & 2\alpha\sin(q_x a)\sin(q_y a) \\ 2\alpha\sin(q_x a)\sin(q_y a) & 2\alpha[1-\cos(q_x a)\cos(q_y a)] \end{bmatrix}$$

b) For propagation in the $\hat{x}$ direction $\vec{q} = q\hat{x}$ and $\omega_{TA} = \omega_{LA} = \sqrt{\frac{\alpha a}{M}}q$ and the eigenvectors are:

$$\begin{bmatrix} u_x \\ u_y \end{bmatrix}_{TA} = A\begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \begin{bmatrix} u_x \\ u_y \end{bmatrix}_{LA} = A\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

For propagation in the $(\hat{x}+\hat{y})/\sqrt{2}$ direction, $\vec{q} = q\,(\hat{x}+\hat{y})/\sqrt{2}$. If you calculate the frequencies, one will come out to be zero for all magnitudes of the wavevector. This is an indication of the fact there is no TA mode that propagates in the $(\hat{x}+\hat{y})/\sqrt{2}$ direction. The LA mode frequency in the $(\hat{x}+\hat{y})/\sqrt{2}$ direction is, $\omega_{LA} = \sqrt{\frac{2\alpha a}{M}}q$ and the eigenmode is $\begin{bmatrix} u_x \\ u_y \end{bmatrix}_{LA} = A\begin{bmatrix} 1 \\ 1 \end{bmatrix}$.

Problem 8.2: (Time-dependent effective mass equation)

a) The answer is,

$$\phi(\vec{r},t) = \exp\left[-\frac{i}{\hbar}\int_0^t \left(E(t') + e\vec{E}\,.\,\vec{r}\right)dt'\right]$$

The solution can be checked by direct substitution is the effective mass equation,

$$\left[E_n\left(\vec{k}_o - i\nabla\right) + e\vec{E}.\,\vec{r}\right]\phi(\vec{r},t) = i\hbar\,\frac{\partial\phi(\vec{r},t)}{\partial t}$$

b) Upon substitution in the effective mass equation, the assumed solution gives,

$$E(t) = E_n\left(\vec{k}_o - \frac{e\vec{E}}{\hbar}t\right)$$

Therefore, the energy of the solution is time dependent and changes with time as the wavevector (or the crystal momentum) changes.

Problem 8.3: (Effective mass equation and probability current)

a) Note that irrespective of the details of the energy band dispersion relation, a plane wave is always an eigenfunction of the $E_n\left(\vec{k}_o - i\nabla\right)$ operator,

$$E_n\left(\vec{k}_o - i\nabla\right)\phi(\vec{r},t) = E_n\left(\vec{k}_o - i\nabla\right)e^{i\vec{q}.\vec{r}} = \sum_j E_n\left(\vec{R}_j\right)e^{i\left(\vec{k}_o - i\nabla\right).\vec{R}_j}e^{i\vec{q}.\vec{r}}$$

$$= \sum_j E_n\left(\vec{R}_j\right)e^{i\vec{k}_o.\vec{R}_j}e^{i\vec{q}.\left(\vec{r}+\vec{R}_j\right)} = E_n\left(\vec{k}_o + \vec{q}\right)e^{i\vec{q}.\vec{r}}$$

So a plane wave has to satisfy the equation,

$$\left[\hat{E}_c\left(\vec{k}_o - i\nabla\right)\right]\phi(\vec{r}) = E\,\phi(\vec{r})$$

with energy eigenvalue equal to $E_c\left(\vec{k}_o + \vec{q}\right)$, which equals,

$$E_c + \frac{\hbar^2 (q_x)^2}{2m_x} + \frac{\hbar^2 (q_y)^2}{2m_y} + \frac{\hbar^2 (q_z)^2}{2m_z}$$

b) $\psi(\vec{r}) = \phi(\vec{r})\psi_{c,\vec{k}_o}(\vec{r}) = e^{i\vec{q}.\vec{r}}\psi_{c,\vec{k}_o}(\vec{r})$

$$\Rightarrow \psi\left(\vec{r}+\vec{R}\right) = \phi\left(\vec{r}+\vec{R}\right)\psi_{c,\vec{k}_o}\left(\vec{r}+\vec{R}\right) = e^{i\left(\vec{k}_o+\vec{q}\right).\vec{r}}\phi(\vec{r})\psi_{c,\vec{k}_o}(\vec{r})$$

c) $$J_\alpha(\vec{r}) = \sum_\beta \phi^*(\vec{r})\frac{\hbar}{2im_{\alpha\beta}}\partial_\beta\phi(\vec{r}) + c.c.$$

$$\Rightarrow J_x(\vec{r}) = \phi^*(\vec{r})\frac{\hbar}{2im_x}\partial_x\phi(\vec{r}) + c.c = \frac{\hbar q_x}{m_x}$$

$$\Rightarrow J_y(\vec{r}) = \phi^*(\vec{r})\frac{\hbar}{2im_y}\partial_y\phi(\vec{r}) + c.c = \frac{\hbar q_y}{m_y}$$

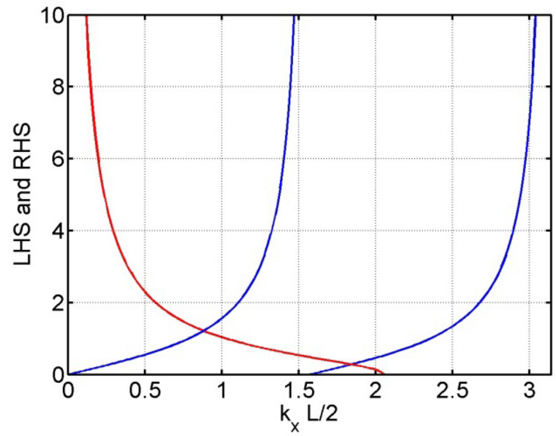
$$\Rightarrow J_z(\vec{r}) = \phi^*(\vec{r})\frac{\hbar}{2im_z}\partial_z\phi(\vec{r}) + c.c = \frac{\hbar q_z}{m_z}$$

Problem 8.4:

a) The transcendental equation to be solved are:

$$\begin{cases} \tan\left(\frac{k_x L}{2}\right) = \frac{m_{x1}}{m_{x2}}\frac{\alpha}{k_x} = \frac{m_{x1}}{m_{x2}}\frac{\sqrt{\frac{2m_{x2}}{\hbar^2}\Delta E_c - \frac{m_{x2}}{m1}k_x^2}}{k_x} \\ -\cot\left(\frac{k_x L}{2}\right) = \frac{m_{x1}}{m_{x2}}\frac{\alpha}{k_x} = \frac{m_{x1}}{m_{x2}}\frac{\sqrt{\frac{2m_{x2}}{\hbar^2}\Delta E_c - \frac{m_{x2}}{m_{x1}}k_x^2}}{k_x} \end{cases}$$

These are slightly modified from the ones in the lecture handouts because the effective masses in the x-direction in the well and the barrier regions are different. We calculate the value of k_x for which the RHS goes to zero. This comes out to be, $k_x L/2 = 2.05$. This is bigger than $\pi/2$ but smaller than π so there are two bound states.



b) The RHS and the LHS of the transcendental equations are plotted. The intersections give the quantized values of k_x. The corresponding energies are:

$E_1 = 27.7$ meV

$E_2 = 121.3$ meV

c) $n = \frac{\sqrt{m_y m_z}}{\pi \hbar^2} KT \log\left(1 + e^{(E_f - E_1 - E_{c1})/KT}\right) + \frac{\sqrt{m_y m_z}}{\pi \hbar^2} KT \log\left(1 + e^{(E_f - E_2 - E_{c1})/KT}\right)$

d) Assume T=300K (room temperature). Plot the RHS as a function of the Fermi level and see which value of the Fermi level gives you the electron density on the LHS. This method yields $E_f - E_{c1} = 53.4$ meV.