ECE 456 - Problem Set 3 (Part 2)

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TOTAL: $\frac{25}{25}$

Well done,
David and Phillip!

Problem 3

Q3: $\frac{10}{10}$

(a) Given the geometry and interaction rules stated, the interaction matrices $[H]_{nm}$ are zero except for

$$[H]_{nn} = \begin{bmatrix} E_0 & t_i \\ t_i & E_0 \end{bmatrix}$$
$$[H]_{n,m*} = \begin{bmatrix} t_A & 0 \\ 0 & t_B \end{bmatrix}$$

where $m*$ corresponds to any of the four nearest neighbor square-shaped unit cells to cell n. For cell n, let cell a be above, cell b be to the right, cell c be below, and cell d be to the left. Given that each cell is spaced a length a apart, the associated phase factors for nonzero H_{nm}, $e^{i\vec{k}\cdot(\vec{d_m}-\vec{d_n})}$, are then:

$$\begin{aligned} (n): &\quad 1 \\ (a): &\quad e^{ik_y a} \\ (b): &\quad e^{ik_x a} \\ (c): &\quad e^{-ik_y a} \\ (d): &\quad e^{-ik_x a} \end{aligned}$$

with $\vec{k} = k_x\hat{x} + k_y\hat{y}$. The Bloch matrix then follows:

$$\begin{aligned} [h(\vec{k})] &= \sum_m [H]_{nm} e^{i\vec{k}\cdot(\vec{d_m}-\vec{d_n})} \\ &= \begin{bmatrix} E_0 + t_A\left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}\right) & t_i \\ t_i & E_0 + t_B\left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}\right) \end{bmatrix} \\ &= \begin{bmatrix} E_0 + 2t_A\left(\cos(k_x a) + \cos(k_y a)\right) & t_i \\ t_i & E_0 + 2t_B\left(\cos(k_x a) + \cos(k_y a)\right) \end{bmatrix} \end{aligned}$$

(b) To find the E-$\vec{k}$ relationship in terms of cosine functions, we must first find h_0 in terms of trigonometric functions. We will require the following trigonometric identities to do so:

$$\sin(\alpha \pm \beta) = \sin(\alpha)\cos(\beta) \pm \sin(\beta)\cos(\alpha) \tag{1}$$

$$\cos(\alpha \pm \beta) = \cos(\alpha)\cos(\beta) \mp \sin(\alpha)\sin(\alpha) \tag{2}$$

$$1 = \sin^2(\theta)\cos^2(\theta), \tag{3}$$

as well as the following general sine/cosine properties:

$$\begin{aligned} \cos(\theta) &= \cos(-\theta) \\ \sin(\theta) &= -\sin(-\theta). \end{aligned} \tag{4}$$

First we can rewrite the exponentials in h_0 using Euler's identity:

$$h_0 = -t_c\left(1 + \cos(-k_x a - k_y b) + i\sin(-k_x a - k_y b) + \cos(-k_x a + k_y b) + i\sin(-k_x a + k_y b)\right)$$

Using identities (1) and (2), we can expand this relationship further.

$$h_0 = -t + c\big(1 + \cos(-k_x a)\cos(-k_y b) - \sin(-k_x a)\sin(-k_y b) + i\sin(-k_x a)\cos(-k_y b) + i\sin(-k_y b)\cos(-k_x a) \\ + \cos(k_y b)\cos(k_x a) + \sin(k_y b)\sin(k_x a) + i\sin(k_y b)\cos(k_x a) - i\sin(k_x a)\cos(k_y b)\big)$$

Here we can use the properties from (4) to reduce this equation. Since $|h_0|^2 = h_0 h_0^*$, we also obtain a simple expression for h_0^*.

$$h_0 = -t_c\left(1 + 2\cos(k_x a)\cos(k_y b) - 2i\sin(k_x a)\cos(k_y b)\right)$$
$$h_0^* = -t_c\left(1 + 2\cos(k_x a)\cos(k_y b) + 2i\sin(k_x a)\cos(k_y b)\right)$$

We can now find $|h_0|^2 = h_0 h_0^*$:

$$h_0 h_0^* = 1 + 4\cos(k_x a)\cos(k_y b) + 4\cos^2(k_y b)$$

From this, we can finally obtain an expression for $E(\vec{k})$:

$$E(\vec{k}) = E_0 \pm t_c\sqrt{1 + 4\cos(k_x a)\cos(k_y b) + 4\cos^2(k_y b)} \tag{5}$$

Problem 4

Q4: $\frac{13}{13}$

(a) We can substitute (from the assignment) equation (24) into equation (23):

$$\sum_k i\hbar\frac{\partial}{\partial t}c_k(t)\phi_k(x)e^{-i[E(k)/\hbar]t} = \sum_k c_k(t)\hat{H}_0\phi(x)e^{-i[E(k)/\hbar]t} \tag{6}$$

$$+\sum_k c_k(t)U_s(x,t)\phi_k(x)e^{-i[E(k)/\hbar]t} \tag{7}$$

We can partially evaluate the derivative on the left hand side:

$$\frac{\partial}{\partial t}c_k(t)\phi_k(t)e^{-i[E(k)/\hbar]t} = \frac{\partial c_k(t)}{\partial t}\phi_k(t)e^{-i[E(k)/\hbar]t} - \frac{i}{\hbar}c_k(t)E(k)\phi_k(x)e^{-i[E(k)/\hbar]t}$$

Expanding the rightmost term out into the summation, we get the expression $\sum_k c_k(t)E(k)\phi_k(x)e^{-i[E(k)/\hbar]t}$. Since $\hat{H}_0\phi_k(x) = E(k)\phi_k(x)$, we can see that this cancels out the term with $\hat{H}_0$ in our first substition (7), and we get the final differential equation:

$$\sum_k c_k(t)U_s(x,t)\phi_k(x)e^{-i[E(k)/\hbar]t} = \sum_k i\hbar\frac{\partial c_k(t)}{\partial t}\phi_k(x)e^{-i[E(k)/\hbar]t}$$

(b)

$$\sum_k c_k(t)\left[\int \phi^*_{k_f}(x)U_s(x,t)\phi_k(x)\,dx\right]e^{-i[E(k)/\hbar]t} = \sum_k i\hbar\frac{\partial c_k(t)}{\partial t}\left[\int \phi^*_{k_f}(x)\phi_k(x)\,dx\right]e^{-i[E(k)/\hbar]t}$$

$$\sum_k c_k(t)I_{k_f k}e^{-i[E(k)/\hbar]t} = \sum_k i\hbar\frac{\partial c_k(t)}{\partial t}\delta_{k_f k}e^{-i[E(k)/\hbar]t}$$

$$\sum_k c_k(t)I_{k_f k}e^{-i[E(k)/\hbar]t} = i\hbar\frac{\partial c_k(t)}{\partial t}e^{-i[E(k)/\hbar]t}$$

where $I_{k_f k}$ is as defined in the assignment and $\delta_{k_f k}$ is the Kronecker delta.

(c) Starting with the initial equation

$$\sum_k c_k(t)I_{k_f k}e^{-i[E(k)/\hbar]t} = i\hbar\frac{\partial c_{k_f}(t)}{\partial t}e^{-i[E(k_f)/\hbar]t}$$

Since we approximated that $c_k = 1$ only when $k = k_i$ and is 0 otherwise, we can simplify the sum on the left hand side to a single element, and divide out the exponentials.

$$I_{k_f k_i}e^{i[-E(k_i)+E(k_f)/\hbar]t} = i\hbar\frac{\partial c_k(t)}{\partial t}$$

Defining a new symbol $\Lambda = [E(k_f) - E(k_i)]/\hbar$, we can simplify the equation to its final form.

$$I_{k_f k_i} e^{i\Lambda t} = i\hbar \frac{\partial c_k(t)}{\partial t} \tag{8}$$

(d)

$$\int \frac{\partial c_{k_f}(t)}{\partial t} = \frac{1}{i\hbar} I_{k_f k_i} \int e^{i\Lambda t}$$

$$c_{k_f}(t) = \frac{1}{i\hbar} I_{k_f k_i} \frac{1}{i\Lambda} e^{i\Lambda t} + C$$

$$c_{k_f}(t) = \frac{1}{i\hbar} I_{k_f k_i} e^{i\Lambda t/2} \left[\frac{1}{i\Lambda} e^{i\Lambda t/2} + C e^{-i\Lambda t/2} \right]$$

Let $C = -\frac{1}{i\Lambda}$. We then have:

$$c_{k_f}(t) = \frac{1}{i\hbar} I_{k_f k_i} e^{i\Lambda t/2} \frac{1}{i\Lambda} \left[e^{i\Lambda t/2} - e^{-i\Lambda t/2} \right]$$

$$c_{k_f}(t) = \frac{1}{i\hbar} I_{k_f k_i} e^{i\Lambda t/2} \frac{\sin(\Lambda t/2)}{\Lambda/2}.$$

Hi David and Phillip,
Actually, this isn't quite rigorous, but no marks off!!
—Alan

(e) To generate the points, we used a simple MATLAB script:

```
% Parameters to change
N_D = 4.7e15;
N_A = 1.6e15;

% Logarithmic tick marks
T = [ 5 6 7 8 9 10 20 30 40 50 60 70 80 90 100 200 300 ];

gamma = 1.057e7 * T / sqrt(N_D - N_A);

mu_n_first = 21.15e17 * (T.^(3/2) / (N_D + N_A));
mu_n_last = (log(1 + gamma.^2) - (gamma.^2 ./ (1 + gamma.^2)));

mu_n = mu_n_first ./ mu_n_last;

for n = 1 : length(T)
    fprintf("T = %dK: %f\n", T(n), mu_n(n));
end
```

Plotting on the provided graph, gives the following:

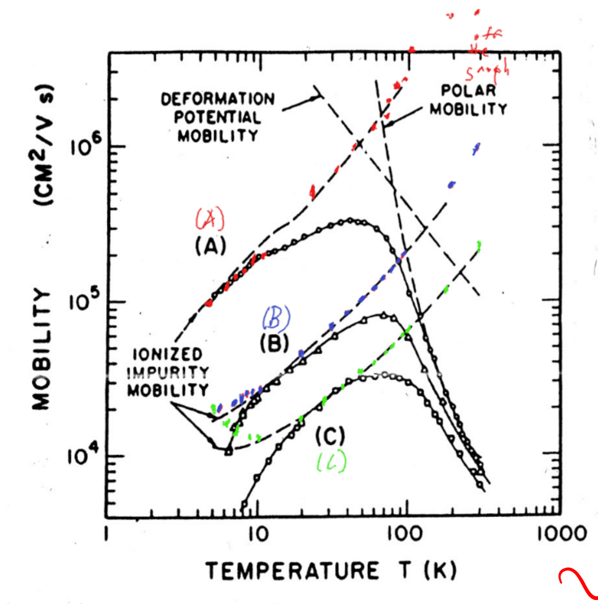

Figure 1. *Graph of electron mobility in GaAs.*

It's clear that our calculated results match up well with the theoretical results.