Physics 5491
Condensed Matter Physics I
Problem Set 6
Due: Thursday, Oct. 18

6.1 Problem 2, Chapter 8 of A&M, Pg. 149.

6.2 Consider a two-dimensional solid with the periodicity of a square Bravais lattice (i.e. a lattice with primitive vectors $\vec{a}_1 = a\hat{x}$ and $\vec{a}_2 = a\hat{y}$).

(a) Show that the first Brillouin zone for this solid consists of wave vectors $\vec{k} = (k_x, k_y)$ for which

$$-\frac{\pi}{a} < k_x \leq \frac{\pi}{a} \quad \text{and} \quad -\frac{\pi}{a} < k_y \leq \frac{\pi}{a}.$$

(b) Show that if electrons in this solid experience a weak periodic potential then the Fourier component of the electron wave function $c_{\vec{k}_1}$ with $\vec{k}_1 = (\pi/a, \pi/a)$ will be strongly coupled to three other Fourier components. What are the wave vectors of these three other components, and what are the reciprocal lattice vectors $\vec{K}$ which connect them to $\vec{k}_1$ and to each other?

Now assume the periodic potential has the following form,

$$U(\vec{r}) = \Delta \sin\frac{2\pi x}{a} \sin\frac{2\pi y}{a}.$$

(c) Obtain the Fourier components of $U(\vec{r})$,

$$U_{\vec{K}} = \frac{1}{v}\int_{cell} U(\vec{r}) e^{-i\vec{K}\cdot\vec{r}}\, d^2r.$$

(d) Show that for this potential, because some of the $U_{\vec{K}}$'s vanish, the component $c_{\vec{k}_1}$ is strongly coupled to only *one* other component $c_{\vec{k}_2}$. What is $\vec{k}_2$?

(e) Obtain a closed 2×2 system of equations for $c_{\vec{k}_1}$ and $c_{\vec{k}_2}$ starting with the Schrödinger equation in momentum space,

$$(\mathcal{E}(\vec{q}) - \mathcal{E})c_{\vec{q}} + \sum_{\vec{K}} U_{\vec{K}} c_{\vec{q}-\vec{K}} = 0$$

for $\vec{q} = \vec{k}_1$ and $\vec{q} = \vec{k}_2$ and assuming that all the $c_{\vec{q}}$ with $\vec{q} \neq \vec{k}_1, \vec{k}_2$ are of order U (and thus can be ignored at lowest order).

(f) Solve the equations obtained in (e) to find the energy bands near the point $\vec{k}_1$.

(g) Sketch the energy bands found in (f) for wave vectors $\vec{k} = k(1,1)$ and $0 \leq k \leq \pi/a$. Indicate the magnitude of the energy gap at the point $\vec{k}_1 = (\pi/a, \pi/a)$.

6.3 Consider a two dimensional lattice with primitive vectors

$$\vec{a}_1 = a\hat{x}, \qquad \vec{a}_2 = \frac{a}{2}\hat{x} + a\hat{y}.$$

(a) Obtain primitive vectors for the reciprocal lattice. (You can do this using the three-dimensional expressions for $\vec{b}_i$ and finding $\vec{b}_1$ and $\vec{b}_2$ using $\vec{a}_3 = \hat{z}$).

(b) Carefully sketch the first and second Brillouin zones for this lattice.

(c) Determine the areas of the first and second Brillouin zones.