1. Tight-binding model for $d = 2$ square lattice.

Here we will consider and solve a tight-binding model on the two-dimensional square lattice. The lattice sites have position $\vec{r} = n_x a \hat{x} + n_y a \hat{y}$, where $n_x = 1, \ldots, N_x$ and $n_y = 1, \ldots, N_y$, for a total of $N = N_x N_y$ lattice sites. We assume periodic boundary conditions, so that $\vec{r}$, $\vec{r} + N_x a \hat{x}$, and $\vec{r} + N_y a \hat{y}$ are all considered to be the same site.

Just as for the one-dimensional example in lecture, we consider a single orbital on each site, so that the state $|\vec{r}\rangle$ describes an electron localized on site $\vec{r}$. (As usual, we don’t worry about spin explicitly, and only take it into account at the end by saying that each state can accommodate up to two electrons.) We assume $\langle \vec{r} | \vec{r}' \rangle = 1$ if $\vec{r} = \vec{r}'$, and $\langle \vec{r} | \vec{r}' \rangle = 0$ otherwise.

We consider the Hamiltonian

$$H = -t \sum_{\vec{r}} \left[ |\vec{r}' + a \hat{x}\rangle \langle \vec{r}' | + |\vec{r}' + a \hat{y}\rangle \langle \vec{r}' | + H.c. \right],$$

where $t > 0$, and “H.c.” stands for Hermitian conjugate (as we used it in class). This Hamiltonian describes tunneling between nearest-neighbor sites of the square lattice, in both horizontal and vertical directions. The sum over $\vec{r}$ means, more explicitly,

$$\sum_{\vec{r}} = \sum_{n_x=1}^{N_x} \sum_{n_y=1}^{N_y}.$$

(1)

Since we are in two dimensions, we need to consider two discrete translation operators,

$$T_x |\vec{r}\rangle = |\vec{r} + a \hat{x}\rangle$$

$$T_y |\vec{r}\rangle = |\vec{r} + a \hat{y}\rangle.$$  

(2)

(3)

(4)

Proceeding analogously to our discussion of $d = 1$ in class, we define states

$$|\vec{k}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{i \vec{k} \cdot \vec{r}} |\vec{r}\rangle.$$  

(5)

(a) Show that $T_x |\vec{k}\rangle = e^{-ik_x a} |\vec{k}\rangle$ and $T_y |\vec{k}\rangle = e^{-ik_y a} |\vec{k}\rangle$.

(b) One way to express periodic boundary conditions is that $T_x^{N_x} |\vec{k}\rangle$ and $T_y^{N_y} |\vec{k}\rangle$ have to act as the identity operator on any state – that is, if you translate all the way around the system (say $N_x$ translations in the $x$-direction), you get back where you started. In particular, $T_x^{N_x} |\vec{k}\rangle = T_y^{N_y} |\vec{k}\rangle = |\vec{k}\rangle$. Use this, and the results of part (a) above, to show that periodic boundary conditions imply that

$$\vec{k} = \frac{2\pi n_x}{a N_x} \hat{x} + \frac{2\pi n_y}{a N_y} \hat{y}.$$  

(6)

for any integers $n_x, n_y$.

(c) Show that $|\vec{k} + (2\pi/a) \hat{x}\rangle = |\vec{k} + (2\pi/a) \hat{y}\rangle = |\vec{k}\rangle$. (Therefore, $\vec{k}$ is only defined modulo the two primitive reciprocal lattice vectors $(2\pi/a) \hat{x}$ and $(2\pi/a) \hat{y}$.)

(d) Show by brute force calculation that $|\vec{k} |\vec{k}\rangle = 1$ if $\vec{k} = \vec{k}'$, and $|\vec{k} |\vec{k}'\rangle = 0$, otherwise.

(e) Using the results of part (b) and part (c), find the total number of distinct states $|\vec{k}\rangle$. In part (d) you showed that the $|\vec{k}\rangle$’s are an orthonormal set of vectors. The $|\vec{k}\rangle$’s also form a complete basis ... how do you know this, just from the total number of states $|\vec{k}\rangle$?
(f) Show that

$$ |\vec{r}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k} \cdot \vec{r}} |\vec{k}\rangle, \quad (7) $$

where the sum is over the allowed distinct values of $\vec{k}$. (Remember that we showed the analogous statement in $d = 1$ in class. One way to proceed is by generalizing the argument we used in class.)

(g) Plug Eq. (7) into the Hamiltonian, and show that

$$ H = \sum_{\vec{k}} \epsilon_{\vec{k}} |\vec{k}\rangle \langle \vec{k}|, \quad (8) $$

where

$$ \epsilon_{\vec{k}} = -2t \left[ \cos(k_x a) + \cos(k_y a) \right]. \quad (9) $$

(h) Draw the Fermi surface for the following values of $\epsilon_F$: $\epsilon_F = 0$, $\epsilon_F = -4t + \delta$, $\epsilon_F = 4t - \delta$. Here, $\delta > 0$ is small compared to $t$. In addition to drawing the Fermi surface, indicate also those regions of $\vec{k}$-space filled by electrons and those that are empty. To draw these Fermi surfaces you first need to draw the region of the $k_x$-$k_y$ plane containing the allowed values of $\vec{k}$. (For instance, in one dimension, we chose the interval $k \in [-\pi/a, \pi/a]$.) Then in each case, the Fermi surface will be a curve (or perhaps a set of curves) inside this region.