ph 135

Problem set - 6

Due: Nov. 26th by 5pm in TA box (happy thanksgiving!).

1. Tight binding energy eigenvalues (Filling in from last problem set).

   Recall that in PS5 problem 2 we had an overlap matrix (we neglect further than nearest neighbor overlaps):

$$M_{nm} = \delta_{nm} + e^{-\lambda a}\left(1 + \frac{\lambda a}{2}\right)\delta_{|n-m|,1} \tag{1}$$

   And h_{nm} which is:

$$h_{nm} = -|\epsilon| M_{nm} + \frac{mV_0^2}{2\hbar^2} e^{-\lambda a}\delta_{|n-m|,1}. \tag{2}$$

   with $\epsilon = -\frac{mV_0^2}{2\hbar^2}$, and $\lambda = \frac{mV_0}{\hbar^2}$.
   Find the tight-binding energy eigenvalues, which are the eigenvalues of the matrix:

$$h_{eff} = M^{-1/2} h M^{-1/2}. \tag{3}$$

   Note that the eigenstates are also momentum eigenstates, so the eigenvalues should be given as a function of momentum.

2. Graphene tight binding.

   Consider an atomic honeycomb lattice - tiled hexagones with atom sites at the vertices - with the distance between nearest neighbors being a. Let us find the tight-binding band structure of this lattice.

   (a) What are the basis vectors, $\vec{a}_1, \vec{a}_2$ of the lattice? Note that there are two atoms in each unit cell.

   (b) Assume that each atom supports a single orbital, which is orthogonal to orbitals in other atoms. Denote the amplitude of the orbital on site A and B of the unit cell at $\vec{r}$ as $\psi_{\vec{r}}^{A,B}$. Assume that electrons can hop between nearest-neighbor atoms with amplitude $-t$. Write down the time-independent Schroedinger equation for the amplitudes $\psi_{\vec{r}}^{A,B}$. Note that this equation will connect $\psi_{\vec{r}}^{A,B}$ with $\psi_{\vec{r}\pm\vec{a}_i}^{A,B}$ with $i = 1, 2$.

   (c) Solve the tight-binding Schroedinger equation you found above. Hint: use a plane wave ansatz of the form $\begin{pmatrix} u \\ v \end{pmatrix} e^{i\vec{p}\cdot\vec{r}}$. What are the energy eigenvalues for each momentum $\vec{p}$? What are $\begin{pmatrix} u \\ v \end{pmatrix}$ as a function of momentum?

   (d) The honeycomb spectrum contains two points with double degeneracy and energy zero. What is the momentum $\vec{p}_{K,K'}$ of these two points? Expand the energy vs. momentum function about these points, and show that $\epsilon_{\vec{p}} \propto |\vec{p} - \vec{p}_K|$ about $\vec{p}_K$ and similarly for K'.

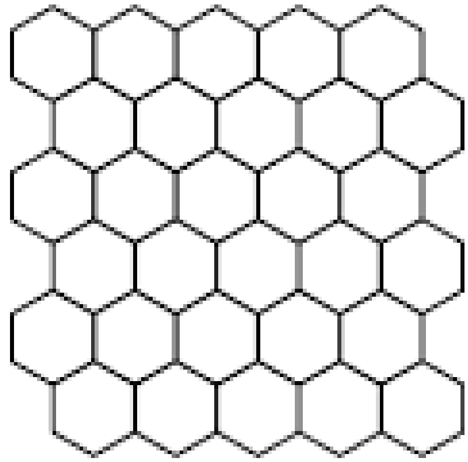

FIG. 1: A honeycomb lattice, which describes graphene.