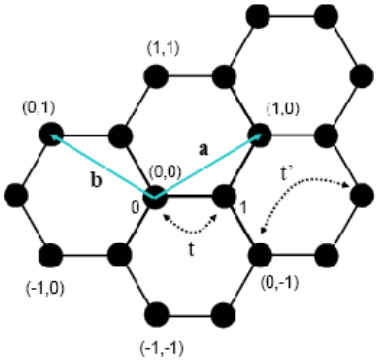
**Phys 231, Fall 2007, Homework 5, due November 26**

(4 points per each problem)

1. A&M 8.2
2. Consider a 2 dimensional simple square crystal with a divalent atom per unit square. I.e., there are two valence electrons contributed by each atom that occupies a square of dimensions $a \times a$.
   (a) In the free electron approximation, what is the Fermi momentum $k_F$? In particular, show that $k_F > \pi/a$, $1.1\ \pi/a$, and $k_F < \sqrt{2}\ \pi/a$.
   (b) Draw the reciprocal lattice, including your origin of choice, its nearest neighbor lattice points, and its next nearest neighbor lattice points. Draw Brillouin zones (BZ's) for all the reciprocal lattice points that you included. Then, draw in the Fermi surface in the free electron approximation. Do this in the repeated zone scheme, i.e., draw the free electron Fermi surface around the origin, and then duplicate it by translating its center to each lattice point that you included.
   (c) Now look at the zone corresponding to the origin of your choice. Sketch all free electron dispersions that are folded into this zone along two vertical lines defined by $k_x = 0.9\ \pi/a$ and $k_x = \pi/a$. In this sketch, take your x-axis to be $k_y$ from $-\pi/a$ to $\pi/a$. In the sketch, indicate the Fermi energy position, and the degeneracy of each dispersion (you can exclude spin). Now, let's turn on potential $V(K=2\pi/a)$ (and necessarily $V(K=-2\pi/a)$) and define $\Delta \equiv |V(2\ \pi/a)|$. Assume that $\Delta$ is a very small number compared to any energy separation between dispersion curves in your plots, but still a finite number. To the leading order in $\Delta$, explain quantitatively what happens to the dispersion curves, and plot new dispersion curves.
   (d) Using your results of (c) and the fact that Fermi surface is orthogonal to the BZ face for a weak potential, as we covered in class, determine the geometry of Fermi surface(s) under the weak crystal potential. Explain why the Fermi surface can be thought of a small "cigar" shaped electron pocket and a small "circle" (or "diamond") shaped hole pocket. Explain why there should be a definite relationship between the area of the "cigar" shape and the area of the "circle" shape, and state what is the relationship.
3. As discussed in class, the electronic structure of high-temperature superconductors (HTSC's) can be discussed essentially within the 2-dimensional square lattice approximation, in which the unit formula is $CuO_2$. In the square unit cell, Cu occupies the vertices, each O occupies the center of nearest neighbor Cu ions. Furthermore, in the so-called un-doped parent compound of HTSC, the valence configuration of Cu is $3d^9$, while the valence configuration of O is $(2sp)^8$. (1) Explain, using Wilson's rule, whether a HTSC should be a metal or an insulator. (2) Let's consider the fact that the HTSC parent compound has an "anti-ferromagnetism," (AFM) namely, each neighboring Cu spin points in opposite directions. This affects the periodicity of the crystal. Sketch a portion of the crystal and indicate the unit cell with and without consideration of the AFM. In the wave vector space, indicate the first Brillouin zone for each case. According to Wilson's rule, can this AFM state be an insulator? [Note: none of these answers actually have direct bearing

on the real physics of HTSC, as an un-doped HTSC is a large-gap insulator even without being an AFM and its gap size far exceeds that of an AFM in the 2nd scenario.]

4. The crystal structure of graphene is shown below. Also, the basis vectors, $\vec{a}, \vec{b}$, are defined. Each carbon atom has 4 valence electrons, 3 of which form strong σ bonds with neighboring carbon atoms by forming covalent $(sp)^3$ bonding, as arising from an s, $p_x$, and $p_y$ orbitals. We are concerned not with these electrons, but with the last electron that occupies $p_z$ orbital. The hopping matrix element for this electron is defined as t and t': $\langle A|H|B\rangle = t$, if *(A,B)* are $p_z$ orbitals for the nearest neighbor carbon atoms, and $t'$, if *(A,B)* are $p_z$ orbitals for the next nearest neighbor carbon atoms. Let's assume that all other matrix elements of *H* is zero.




(1) Write down the explicit forms of $\vec{a}, \vec{b}$. (choose x and y axes to get neat answers in (4))

(2) Assume a tight-binding wave function for the eigen-state:
$|\psi\rangle = \sum_{l,m}[u|lm,0\rangle + v|lm,1\rangle]\exp(i\vec{k}\cdot\vec{R}_{lm})$ (0, 1 are basis indices)
Here, $lm$ are indices for Bravais lattice vectors (some of which are shown in the diagram). Show that the secular equation $H|\psi\rangle = \epsilon(\vec{k})|\psi\rangle$ reduces to a 2x2 matrix equation involving matrix of the form $\begin{bmatrix} t'B & tA^* \\ tA & t'B \end{bmatrix}$. Identify the form of $A$ and $B$.

(3) Show that the eigen value $\epsilon(\vec{k})$ is gven by $t'f(\vec{k}) \pm t\sqrt{3+f(\vec{k})}$ where $f(\vec{k}) = 2\left(\cos(\vec{k}\cdot\vec{a}) + \cos(\vec{k}\cdot\vec{b}) + \cos\left(\vec{k}\cdot(\vec{a}+\vec{b})\right)\right)$. Show that the quantity inside the square root vanishes at 6 corners (three-fold rotations of K and K' points – define two adjacent corners as K and K') of the Brillouin zone in the momentum space and the Fermi energy lies there (assume t < 0, t' < 0 and $|t/t'| \geq 3$)

(4) Show that the matrix equation derived in (2) reduces to a two dimensional relativistic mass-less Dirac Hamiltonian, $c\vec{\sigma}\cdot\vec{p}$, when the wave vector $\vec{p} = \hbar(\vec{k} - \vec{k}_K)$ or $\hbar(\vec{k} - \vec{k}_{K'})$ when $\vec{k}$ is close to K or K' point. What are the values of c for K and K' points? Show that the dispersion $\epsilon(\vec{k})$ describes a cone (Dirac cone). ($\vec{\sigma}$ is Pauli matrix = $(\sigma_x, \sigma_y)$ or $(\sigma_x, -\sigma_y)$, in this case for a "pseudo-spin" corresponding to the sub-lattice (0 or 1) degree of freedom; set t'=0 for this problem)

5. A&M 10.3