Physics 123B: Homework 2

due Friday, January 23, 4pm to Amanda Jones in Kohn Hall 1220

Carbon nanotubes:

Carbon nanotubes are made up of a section of the graphene lattice that has been wrapped up into a cylinder. You can specify the way the lattice is wound up by giving the *winding vector* $\mathbf{W}$. The winding vector must be a Bravais lattice vector, and so can be specified by two integers. The conventional choice is to define

$$\mathbf{W} = m\mathbf{a}_1 + (m+n)\mathbf{a}_2, \tag{1}$$

where m and n are integers, and $\mathbf{a}_1, \mathbf{a}_2$ are the primitive vectors we chose in class. To construct a nanotube, take a graphene lattice and mark the center of one hexagon as the origin. Then draw the winding vector $\mathbf{W}$ from this point to the center of another hexagon. Roll up the sheet perpendicular to $\mathbf{W}$ so that the second hexagon sits exactly on top of the first. You will have constructed a nanotube!

1. Using the graph paper provided (print the included page as a separate sheet), construct a $(10, 10)$ tube (i.e. using scissors and scotch tape!). I recommend photocopying the sheet so you have a backup in case of a mistake!

2. Construct a $(20, 0)$ tube.

3. *Extra credit:* Construct a nanotube with a closed "cap" on one end. The geometry is very interesting!

4. Now back to theory. Let's determine the band structure of a nanotube. To do so, impose periodic boundary conditions on the wavefunction in the direction around the cylinder. Show that this means that $\mathbf{k} \cdot \mathbf{W} = 2\pi l$, where l is an integer.

5. Draw the first Brillouin zone of the 2d system, as in class, indicating (a) the points $\mathbf{K}$ at which $\varepsilon = \epsilon_F$ and (b) the lines given by part (4) for $(m, n) = (3, 3)$ and $(m, n) = (-2, 2)$.

6. Plot the energy versus k_x for the allowed values of k_y in the $(3, 3)$ tube above. Then plot the energy versus versus k_y for the allowed values of k_x in the $(-2, 2)$ tube. For each case, is the nanotube metallic or insulating according to band theory?

7. For which m and n are the Brillouin zone corners allowed wavevectors for a nanotube cylinder? Show that the tubes satisfying this condition are metallic!

8. In reality, one expects that the curvature of the nanotube cylinder affects the tight-binding matrix elements slightly. Consider this effect for the special cases of "armchair" (N, N) tubes and "zig-zag" $(-N, N)$ tubes. In these cases, the curvature effect can be modeled by making the hopping matrix element slightly different $(= t')$ on the vertical links than on the diagonal ones $(= t)$. How does this affect the metallicity of the armchair and zig-zag tubes?