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

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

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 $k \cdot \mathbf{W} = 2\pi l$, 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 $k_y$ 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?