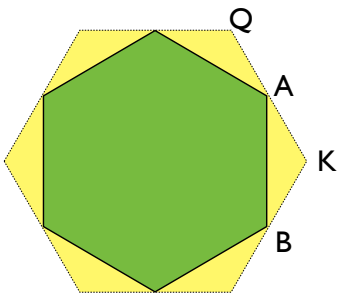
Physics 123B: Final
Due March 14, 2013, 9:30AM

1. Consider the model band structure of graphene from class. Suppose electrons are added to graphene so that the Fermi energy increases from $\epsilon_F = \epsilon_0$ to $\epsilon'_F = \epsilon_0 + \gamma$, where γ is the tight-binding matrix element introduced in class. Find and plot the Fermi surface. How many additional electrons have been added to the material (compared to neutral graphene), per carbon atom?



Recall from the class notes, that the energy spectrum consists of two bands with energy $\epsilon_\pm = \epsilon_0 \pm |f(\mathbf{k})|$. Setting this equal to ϵ'_F, there is a solution only for ϵ_+, corresponding to a Fermi surface in the upper band. It is given by the condition $|f(\mathbf{k})| = \gamma$. Now $f(\mathbf{k}) = -\gamma g(\mathbf{k})$, where

$$g(\mathbf{k}) = e^{ik_y a_0/2}\left[e^{-\frac{3}{2}ik_y a_0} + 2\cos\left(\frac{\sqrt{3}k_x a_0}{2}\right)\right]. \tag{1}$$

The condition for the Fermi surface is then $|g(\mathbf{k})| = 1$, which is equivalent to $|g|^2 = 1$. Evaluating this, we have with a little algebra

$$\left[2\cos\left(\frac{\sqrt{3}k_x a_0}{2}\right) + \cos\left(\frac{3k_y a_0}{2}\right)\right]^2 + \left[\sin\left(\frac{3k_y a_0}{2}\right)\right]^2 = 1. \tag{2}$$

Now multiplying out the squares and using $\cos^2 x + \sin^2 x = 1$, we get

$$4\cos^2\left(\frac{\sqrt{3}k_x a_0}{2}\right) + 4\cos\left(\frac{\sqrt{3}k_x a_0}{2}\right)\cos\left(\frac{3k_y a_0}{2}\right) = 0. \tag{3}$$

This equation factors and clearly has two solutions:

$$\cos\left(\frac{\sqrt{3}k_x a_0}{2}\right) = 0, \qquad \text{or} \qquad \cos\left(\frac{\sqrt{3}k_x a_0}{2}\right) + \cos\left(\frac{3k_y a_0}{2}\right) = 0. \tag{4}$$

The first equation implies $k_x = \pm\frac{\pi}{\sqrt{3}a_0}$. The second one implies $k_x = \pm\frac{2\pi}{\sqrt{3}a_0} \pm \sqrt{3}k_y$ (since $\cos[\pm(\pi \pm x)] = -\cos x$) – here the two sets of $\pm$ signs are independent. These all describe straight lines in the k_x–k_y plane. If we take care to draw these inside the first Brillouin zone,

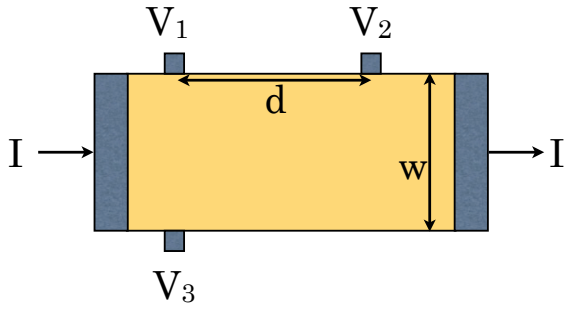
we find that they form the six sides of a hexagon, *inscribed* inside the Brillouin zone! This is shown above.

To get the density of electrons that have been added, we should recognize that this is a *hole* Fermi surface, so the electrons fill the yellow triangles outside the hexagonal fermi surface. The number of added electrons *per unit cell* = 2 (for spin) $\times$ the fraction of the area of the Brillouin zone occupied by these triangles. Since there are two carbon atoms per unit cell, the number of electrons added per carbon is just the fractional area of the zone filled by the yellow triangles. From class, we know the point $K = (\frac{4\pi}{3\sqrt{3}a_0}, 0)$ and $Q = (\frac{2\pi}{3\sqrt{3}a_0}, \frac{2\pi}{3a_0})$. The point A is halfway between K and Q, so $A = (K+Q)/2 = (\frac{\pi}{\sqrt{3}a_0}, \frac{\pi}{3a_0})$, and then $B = (\frac{\pi}{\sqrt{3}a_0}, -\frac{\pi}{3a_0})$. The area of all the yellow triangles is 6 times the area of the triangle ABK. The area of the full Brillouin zone is 6 times the area of the triangle $0KQ$ (0 denotes the origin). So the number of added electrons per carbon atom is the area of ABK divided by the area of $0KQ$. Using area = base $\times$ height/2, we get

$$n_{\text{added}} = \frac{\frac{1}{2} \times \frac{2\pi}{3a_0} \times \frac{\pi}{3\sqrt{3}a_0}}{\frac{1}{2} \times \frac{4\pi}{3\sqrt{3}a_0} \times \frac{2\pi}{3a_0}} = \frac{1}{4}. \tag{5}$$

So there is $1/4$ of an electron added per C atom.

2. A two-dimensional electron gas is patterned into the Hall bar shown in the figure below. The gray rectangles on the ends represent current leads, and the gray squares contacts connected to a voltmeter. A large magnetic field is applied (oriented "up" out of the plane) at very low temperature, so that all electrons are spin polarized and the Fermi level lies between the lowest and first excited Landau level. What is the voltage difference $V_1 - V_3$ and $V_2 - V_3$?



When one Landau level is filled in the bulk, there is a single chiral edge state at the boundary of the sample. Note that since the edge on the top side of the sample is in equilibrium, $V_2 = V_1$, hence $V_1 - V_3 = V_2 - V_3$. The difference between the voltage at the contacts 1 and 3, for example, is given by the argument in class, which concludes that the Hall conductance $G_{xy} = e^2/h$. This means $V_1 - V_3 = V_2 - V_3 = h/e^2 \times I$. (Note that I am not being careful about the sign, and do not expect you to!). In fact the sign should be electron-like.

3. A rotational flow is set up in a superfluid confined between two cylinders. What physical process determines the decay rate of the superflow?

This is determined by the escape of vortex lines, which must move from the inner cylinder to the outer one, passing through the bulk of the superfluid, to cause the flow to decay. This is a thermally activated process, which is very slow at low temperature.

4. Why is heat conduction very efficient in superfluid helium but very poor in a superconductor?

   This is because in helium the normal and superfluid components can both convect, i.e. flow with non-zero *constant* velocity without damping (the normal fluid experiences viscosity, i.e. resistance to velocity *gradients*). In this way the normal component can convect heat even without any net mass flow. In a superconductor, the normal fluid is damped by friction with the lattice, so it only diffuses heat, and there is less and less of it at low temperature to do so.

5. Two Josephson junctions are fabricated identically, except that the barrier region in junction A is twice as thick as that in junction B. Does A or B have the larger critical current? Why?

   The Josephson effect is due to tunneling of electrons across the junction, so the thinner junction, B, will have the larger critical current, as tunneling is more efficient. This also follows from the Ambegaokar-Baratoff formula, since the thinner junction will have lower normal state resistance, hence larger I_c.

6. Find the expected magnetic states in free space for Ni^{2+}, Ni^{3+}, and Ni^{4+} ions, assuming that the 4s electrons are the first to be removed from the free Ni atom. Give the S, L, and J quantum numbers for each case.

   Ni^{2+}=$3d^8$ ↑↓ ↑↓ ↑↓ ↑ ↑

   Ni^{3+}=$3d^7$ ↑↓ ↑↓ ↑ ↑ ↑

   Ni^{4+}=$3d^6$ ↑↓ ↑ ↑ ↑ ↑

   We begin with Ni^{2+}, which has the $3d^8$ configuration. So we should begin by filling the d states, keeping as many electrons as possible unpaired and with spins aligned. For Ni^{2+}, this gives two unpaired electrons, with therefore $S = 1$. To follow Hund's second rule, we maximize L, taking $L_z = 2+1 = 3$ so $L = 3$. From the final Hund's rule, this gives $J = L+S = 4$, since it is a more than half-filled shell. For Ni^{3+}, we get $S = 3/2$, $L = 3$, and hence $J = L+S = 9/2$. For Ni^{4+}, we get $S = 2$, $L = 2$, and $J = L + S = 4$.

7. Give two ways that the exchange coupling J can be measured in a ferromagnet.

   It can be extracted from the Curie-Weiss temperature term in the high temperature magnetic susceptibility. It can also be measured from the spin wave dispersion.

8. Formulate mean field theory for the Heisenberg *antiferromagnet* on the cubic lattice, i.e. $H = +|J| \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$, for $S = 1/2$ spins. In the first two parts, you will need to assume that $\langle \mathbf{S}_i \rangle = +\mathbf{n}$ when $x_i + y_i + z_i$ is an even multiple of the lattice spacing a, and $\langle \mathbf{S}_i \rangle = -\mathbf{n}$, when $x_i + y_i + z_i$ is an odd multiple of the lattice spacing a.

   (a) Find the self-consistent equation for $n = |\mathbf{n}|$.

   Let us call the sites with $x_i + y_i + z_i$ an even multiple of a the A sublattice, and the others the B sublattice. All the nearest neighbors of an A site are B sites. So the

net exchange field on each A site is the sum of those on $z = 6$ neighboring B sites, $\mathbf{h}_A = -|J| \sum_{i=1}^{6} \langle \mathbf{S}_i \rangle_B$. The minus sign occurs because of the antiferromagnetic sign in the Hamiltonian. Now the expectation value is equal to $-\mathbf{n}$ for those B sublattice sites, so the two minus signs cancel and $\mathbf{h}_A = 6|J|\mathbf{n}$. On the B sublattice, the exchange field comes from A sublattice sites, so there is no cancelling minus sign, and $\mathbf{h}_B = -6|J|\mathbf{n}$. We can, without loss of generality, take $\mathbf{n}$ and $\mathbf{h}_A, \mathbf{h}_B$ along the z axis. Then as usual for spin-$1/2$, we have on the A sublattice, $\langle S_i^z \rangle_A = \frac{1}{2} \tanh h_A/(2kT)$. This gives the condition

$$n = \frac{1}{2} \tanh \left(\frac{6|J|n}{2kT} \right). \tag{6}$$

Note that this condition is identical to that for the ferromagnet, but with m replaced by n! We need to check that this also works for the B sublattice. Here we have $\langle S_i^z \rangle_B = \frac{1}{2} \tanh h_B/(2kT)$, which is the same as Eq. (6) but with both sides multiplied by -1, and so is equivalent and consistent.

(b) Find the critical, or Néel, temperature T_N.

Since the above equation is the same as that for the ferromagnet, so is the critical temperature. $T_N = z|J|/(4k) = 3|J|/(2k)$ for $z = 6$.

(c) Find the uniform susceptibility, $\chi = \left. \frac{\partial m^z}{\partial H_z} \right|_{H=0}$, for $T > T_N$. Here H_z is an applied uniform external field along the z axis, and $m^z = \frac{1}{N} \sum_i g\mu_B S_i^z$ is the z-component of the magnetization. You will need to assume here that the average values of the spins on the two sublattices are no longer opposite.

Now let us just assume that $\langle \mathbf{S}_i \rangle = \mathbf{m}_A$ or $\mathbf{m}_B$ if i is on the A or B sublattice, respectively. We have $\mathbf{h}_A = -6|J|\mathbf{m}_B$ and $\mathbf{h}_B = -6|J|\mathbf{m}_A$. Let us again assume that the magnetization and the fields are along the z axis. As in class, we include both the exchange field and the external field. Then we have two conditions:

$$m_A = \frac{1}{2} \tanh \left(\frac{g\mu_B H - 6|J|m_B}{2kT} \right), \qquad m_B = \frac{1}{2} \tanh \left(\frac{g\mu_B H - 6|J|m_A}{2kT} \right). \tag{7}$$

Above the Néel temperature, we expect that the spins vanish in zero applied field, and so we can just expand the $\tanh$ functions to linear order. This gives

$$m_A = \frac{g\mu_B H - 6|J|m_B}{4kT}, \qquad m_B = \frac{g\mu_B H - 6|J|m_A}{4kT}. \tag{8}$$

This linear set of equations has just one solution, for $T \neq T_N$, which is

$$m_A = m_B = \frac{g\mu_B H}{4k(T + T_N)}, \tag{9}$$

using the form of the Néel temperature determined in the previous step. Now the uniform magnetization is $m^z = g\mu_B(m_A + m_B)/2$, which implies

$$\chi = \frac{(g\mu_B)^2}{4k(T + T_N)}. \tag{10}$$

Note that this is the same form as the Curie-Weiss law, but with T_c replaced by $-T_N$, i.e. with a negative Weiss temperature. This fact is often used to diagnose antiferromagnets based on the high temperature susceptibility. Note that because of this sign, the susceptibility does not diverge at T_N.

9. Find the energy versus wavevector dispersion relations for the *two branches* of spin wave modes of the spin-S Heisenberg ferromagnet on the honeycomb lattice.

We need to analyze the spin wave modes in the same way we did for the simple cubic lattice. The basic equation we derived *in real space* is still valid:

$$H|i\rangle = (E_0 + JSz)|i\rangle - JS \sum_{\text{j nn i}} |j\rangle. \tag{11}$$

We can write this in terms of a Schrödinger-like equation by writing

$$|\psi\rangle = \sum_i \psi_i |i\rangle. \tag{12}$$

The wavefunction ψ_i obeys then

$$(E_0 + JSz)\psi_i - JS \sum_{\text{j nn i}} \psi_j = E\psi_i. \tag{13}$$

The difference from the cubic lattice is that now these are sites on the honeycomb lattice, which is not a Bravais lattice, but has two sites per unit cell. So we cannot assume that the magnon is a pure plane wave, but has the Bloch form, with $\psi_i = \psi_A e^{i\mathbf{k}\cdot\mathbf{r}_i}$ if i is on the A sublattice, and $\psi_i = \psi_B e^{i\mathbf{k}\cdot\mathbf{r}_i}$, if i is on the B sublattice.

This is just the exact same problem as the tight-binding model for graphene, except that the orbital energy has been replaced by $\epsilon_0 \to E_0 + JSz$ and the tight-binding matrix element has been replaced by $\gamma \to JS$.

So we can just take over the results! From the notes, we have

$$\begin{aligned} E(\mathbf{k}) &= \epsilon_0 \pm \gamma |g(\mathbf{k})| & (14) \\ &\to E_0 + 3JS \pm JS|g(\mathbf{k})|, & (15) \end{aligned}$$

where we used $z = 3$ for the honeycomb lattice, and $g(\mathbf{k})$ is given in Eq. (1). So defining the magnon energy $\epsilon = E - E_0$, we have

$$\epsilon_\pm(\mathbf{k}) = JS(3 \pm |g(\mathbf{k})|). \tag{16}$$

A good check on this result is that the magnons should always have energies that are greater than or equal to zero, and that there should be Goldstone modes at $k = 0$. Checking Eq. (1), you can check that $g(\mathbf{k} = 0) = 3$, which gives the condition that $\epsilon_-(\mathbf{k} = 0) = 0$, as required!