## Physics 123B: Mid-Term February 4, 2015



Figure 1: Lattice and conventions useful for problem 1.

- 1. Consider the tight-binding model for graphene discussed in class, with hopping  $\gamma$  between nearest-neighbor sites on the honeycomb lattice. Now let us modify this to model a material like boron nitride, BN, which has one type of atom on the A sublattice and another on the B sublattice. In this case, the on-site energy will be different for the two types of sites. Take the energy for the A site to be  $\Delta$ , and the energy for the B site to be  $-\Delta$ .
  - (a) Find the energies of the two bands.

We just need to follow the reasoning we used in class to derive the dispersion, but modifying the on-site energies. We have, for an A sublattice site

$$\hat{H}\psi_R = \epsilon_A \psi_R - \gamma \sum_i \psi_{R+e_i} = \epsilon \psi_R, \qquad (1)$$

with the on-site energy  $\epsilon_A = \Delta$ . Similarly, when R is a B site,

$$\hat{H}\psi_R = \epsilon_B \psi_R - \gamma \sum_i \psi_{R-e_i} = \epsilon \psi_R, \qquad (2)$$

with  $\epsilon_B = -\Delta$ . Now we can plug in the Bloch form  $\psi_i = \psi_{A/B} e^{ik \cdot R}$ , which then gives us

$$\begin{pmatrix} \Delta & f(k) \\ f^*(k) & -\Delta \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \epsilon \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}.$$
(3)

Here, as in class, we have

$$f(k) = -\gamma \sum_{i=1}^{e} e^{ik \cdot e_i} = -\gamma e^{\frac{i}{2}k_y a_0} \left[ e^{-\frac{3}{2}ik_y a_0} + 2\cos\left(\frac{\sqrt{3}k_x a_0}{2}\right) \right].$$
 (4)

Finding the eigenvalues of this matrix, we see that the energy bands are given by

$$\epsilon_{\pm}(k) = \pm \sqrt{|f(k)|^2 + \Delta^2}.$$
(5)

- (b) What is the band gap, i.e. the energy difference between the minimum of the conduction band and the maximum of the valence band, at the K point?
  At the K point, f(K) = 0, so the energy states are just ε<sub>±</sub>(K) = ±|Δ|. Hence the gap is 2|Δ|.
- 2. Please derive (i.e. show how you get it) the density of states for graphene, in terms of energy  $\epsilon$  measured relative to the Dirac point, and velocity v.

The density of states is most easily obtained by the formula  $g(\epsilon) = |dN(\epsilon)/d\epsilon|$ , where  $N(\epsilon)$  is the cumulative density of states, the total number of states, per unit volume, with energy between 0 and  $\epsilon$ . For each spin, and in the vicinity of one Dirac point, these states form a circle in momentum space of radius  $k(\epsilon) = \epsilon/(\hbar v)$ . The number of states inside this sphere is its volume,  $\pi[k(\epsilon)]^2$ , times the density of states in momentum space, which is  $1/(2\pi)^2$ . Hence

$$D(\epsilon) = 4 \times \pi[k(\epsilon)]^2 \times \frac{1}{(2\pi)^2} = \frac{[k(\epsilon)]^2}{\pi} = \frac{\epsilon^2}{\pi \hbar^2 v^2}.$$
 (6)

Taking the derivative, then

$$g(\epsilon) = |D'(\epsilon)| = \frac{2|\epsilon|}{\pi \hbar^2 v^2}.$$
(7)

3. What are three experiments that demonstrate the existence of massless Dirac electrons in graphene?

Some acceptable answers are: ARPES measures the dispersion, tunneling measures the linear DOS of the Dirac points, the unconventional IQHE series  $(\pm 2, \pm 6, \cdot)$ , Klein tunneling.

4. What is the difference between the states at the edge of a Hall bar in the IQHE when  $\sigma_{xy} = 3e^2/h$  versus when  $\sigma_{xy} = e^2/h$ ?

Each edge has 3 chiral edge states when  $\sigma_{xy}=3e^2/h$  and only one edge state when  $\sigma_{xy}=e^2/h$ 

5. Explain why  $\rho_{xx}$  has a peak between Hall plateaus in the IQHE.

Between Hall plateaus, there are "percolating" states in the bulk, which correspond to semiclassical trajectories of the center of mass of the cyclotron orbits drifting along equipotentials that move around the "middle" of the random potential. Equivalently, one can say that one edge state "peels off" the boundary and annihilates with itself to pass from the  $n^{th}$  IQHE state to the  $(n-1)^{th}$  IQHE state.

6. What is the spectrum of Landau levels (i.e. their energies) for the Dirac model of graphene? The energies are ±ħω<sub>c</sub>√n, where n are integers, and (you do not need to get part right in detail) the cyclotron frequency is ω<sub>c</sub> = √2v/ℓ, and ℓ = √ħ/eB is the magnetic length. 7. Explain the observed IQHE values of  $\sigma_{xy}$  in graphene using the edge state picture.

First we need to recall that each edge state contributes  $\pm e^2/h$  to the Hall conductance, with a sign dependent upon the chirality (direction of the velocity) of that edge state. Then we need to understand the edge states for graphene. These are shown in the Figure, showing valley degeneracy (which is broken by the edge) but spin degeneracy is implicit. The positive energy



Landau levels bend up, the negative ones bend down, and the zero energy Landau level splits and half bend up and half bend down. We can see that when the Fermi level is between bulk Landau levels with, say positive energy, as shown, it intersects one spin degenerate edge level from the zeroth Landau level, and two spin degenerate levels for each additional Landau level filled in the bulk. This means that if the Fermi level is  $E_{F1}$  the Hall conductivity is  $2e^2/h$ , while if it is  $E_{F2}$  it increases by  $4e^2/h$  to  $6e^2/h$ , and then to  $10e^2/h$  at  $E_{F3}$  etc. The negative energy edge states disperse in the opposite direction, which implies the opposite sign of Hall conductivity but the same sequence if negative Fermi energies are considered.