Concepts of condensed matter physics Spring 2014

Exercise #5 (due date: 4/07/2014)

1. **The robustness of Dirac fermions in graphene** - In the tutorial we have shown that at low energies (near half-filling) electrons in graphene have a doubly degenerate Dirac spectrum located at two points in the Brillouin zone, namely $K' = \left[0, \frac{4\pi}{3}\right] a^{-1}$ and $K = \left[\frac{2\pi}{\sqrt{3}}, \frac{2\pi}{3}\right] a^{-1}$. An important feature of this dispersion relation is the absence of an energy gap between electrons and holes (which happens only for massless relativistic particles). We also saw that the lattice structure of graphene has unique symmetries (e.g. 3-fold rotational symmetry of the hexagonal lattice). The question is: What symmetry operation protects the Dirac spectrum? Namely, what inherent symmetry in graphene we need to violate in order to destroy the massless Dirac spectrum of the electrons in low energies (i.e. open a band gap).

   a. *Stretching the graphene lattice* - one way to reduce the symmetry of graphene is to stretch its lattice in one direction. In non-stretched graphene the hopping of an electron from a carbon atom to its three nearest-neighbors has equal amplitudes ($t_1 = t_2 = t_3 = t$). Stretching a carbon-carbon bond reduces the hopping element along this bond. So a simple way to take into account the stretching is to keep the hexagonal geometry of graphene fixed but write a tight-binding Hamiltonian with non-equal hopping matrix elements:

   $$H = -\sum_j \sum_{a=1}^{3} t_a \left(c_{A,j}^+ c_{B,j+\delta_a} + \text{H.c.} \right)$$

   where $\delta_3 = [0,1]a$, $\delta_2 = \left[-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right] a$ and $\delta_1 = \left[\frac{\sqrt{3}}{2}, -\frac{1}{2}\right] a$.

   i. Write the tight-binding Hamiltonian for the generic case ($t_1 \neq t_2 \neq t_3$) and solve it numerically (plot the energy bands and the pseudospin for every k in the Brillouin zone)

   ii. What happens to the Dirac cones in homogenous stretching (change the t's but keep them all equal)?

   iii. How are the two Dirac cones affected in the two different cases? Namely $t_1 = t_2 > t_3$ and $t_1 = t_2 < t_3$.

iv. For what values of t_3/t_2 do the Dirac cones gap out? How do you explain the gapping out of the Dirac cones? (remember that these Dirac cones are vortices in k-space such that they can not be continuously deformed into a non-singular configuration of the pseudo spin)

b. *Longer range hopping* - assume a next nearest neighbor hopping term

$$H = -\sum_{<ij>}\sum_{A,B} t'\left(c_{a,i}^+ c_{a,j} + \text{H. c.} \right)$$

Where the <> brackets denote summation over nearest neighbor sites in the **Bravais lattice.** Does the longer range open a gap in the Dirac dispersion?

c. *Directly breaking the symmetry* - Can you think of an additional symmetry breaking that will gap out the Dirac cones?

d. *Disorder* – how small does a local perturbation need to be to open a gap in the dispersion?

2. **Integer Quantum Hall effect in Graphene** – consider the low-energy effective theory of graphene in a magnetic field.

a. Find the Landau-levels in graphene close to half-filling (use the Dirac dispersion relation). Plot the DOS for positive/negative energies.

b. What is the degeneracy of each Landau level? Is it different compared to a quadratic dispersion relation?

c. What is the general structure of the single-particle wave-functions? (use the sub lattice spinor wave function) What is special about the landau level at $n = 0$?

d. Using the relation between the number of filled Landau levels ν and σ_{xy}, plot σ_{xy} as a function of $1/B$ for a given density of electrons. Qualitatively, plot also σ_{xx} on the same plot? What happens at zero density, when the chemical potential is exactly at the neutrality point (half-filling)?

3. **Quantization of inter-layer Hall conductivity** – Consider two parallel two-dimensional conductors (e.g. two layers of graphene separated by an thin insulating buffer). In the presence of a perpendicular magnetic field the generalized conductivity tensor has the following form

$$J_i^a = \sigma_{ij}^{ab} E_j^b$$

where $a = 1,2$ denotes the layer number and J_i^a and E_i^a are the i'th component of the in-plane current density and electric field. Show that the off-diagonal Hall conductivity σ_{xy}^{12} is quantized following the Berry phase arguments presented in class, following these steps:

a. Write the generalized Kubo formula for this off diagonal element.

b. Using a the appropriate toroidal geometry, write this element in terms of derivatives of the ground state with respect to magnetic fluxes.

c. Generalize the Berry phase argument (given in class) to prove that σ_{xy}^{12} is quantized.

4. **A simple tight-binding model for a 2D topological insulator** - Discuss σ_{xy} for spin-less particles a square lattice model that has the following Hamiltonian

$$H = \sum_k \left(\psi_s^+(k) \quad \psi_p^+(k)\right) \widehat{H}(k) \begin{pmatrix} \psi_s(k) \\ \psi_p(k) \end{pmatrix}$$

where

$$\widehat{H}(k) = A\left(\sin k_x \tau_x + \sin k_y \tau_y\right) + \left(m - t\cos k_x - t\cos k_y\right)\tau_z$$

Here the τ's are Pauli matrices acting in the orbital basis.

a. Find the corresponding real-space representation of the tight-binding Hamiltonian. Show that if the p-orbital states belong to the $|l = 1; m_l = 1\rangle$ out of the three p-triplet states then the s-p coupling constant is $\propto \sin k_x + i \sin k_y$.

b. Discuss σ_{xy} as a function of μ

c. Plot the pseudo spin configuration as a function of $e = m/t$ for different values of e_a -- choose them wisely.

d. Assume that the crystal exists only in the for $x < 0$, and for $x > 0$ there is vacuum. Write the Schrodinger equation for the single particle solutions near the Fermi energy and (assume that $m > 0$).

    i. What are the boundary conditions at $x = 0$?

    ii. What are the conditions for the existence of a zero energy solution on the boundary?

    iii. What is the decay length of the wave fundtion?

    iv. What happens to the solution at the critical values of the parameter e?