Concepts of condensed matter physics

Spring 2017

Exercise #1

Due date: 23/04/2017

1. **Adding long range hopping terms** In class 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. An important feature of this dispersion relation is the absence of an energy gap between the upper and lower bands. However, in our analysis we have restricted ourselves to the case of nearest neighbor hopping terms, and it is not clear if the above features survive the addition of more general terms. Write down the Bloch-Hamiltonian when next nearest neighbor and next-next nearest neighbor terms are included (with amplitudes t' and t'' respectively). Draw the spectrum for the case $t = 1, t' = 0.4, t'' = 0.2$. Show that the Dirac cones survive the addition of higher order terms, and find the corresponding low-energy Hamiltonian. In the next question, you will study under which circumstances the Dirac cones remain stable.
2. **The robustness of Dirac fermions in graphene –**We know that the lattice structure of graphene has unique symmetries (e.g. 3-fold rotational symmetry of the honeycomb lattice). The question is: What 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 at low energies (i.e. open a band gap). In this question, consider only nearest neighbor terms.
    a. *Stretching the graphene lattice* - one way to reduce the symmetry of graphene is to stretch its lattice in one direction. Which symmetry is broken in this case?

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:

$$H = -\sum_R \sum_{a=1}^{3} t_a \left(A_R^+ B_{R+\boldsymbol{\delta}_a} + h.c. \right)$$

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

i. Write the Bloch Hamiltonian for the generic case ($t_1 \neq t_2 \neq t_3$) and find the corresponding energy bands and wave functions.
In what follows you can plot the energy bands numerically.

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

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

iv. For what values of t_2/t_1 do the Dirac cones gap out?

v. In class we stated that the Dirac cones can be thought of as vortices in k-space. To make this statement more precise write the Bloch Hamiltonian in the form $h(\vec{k}) = \vec{d} \cdot \vec{\sigma}$, where the σ_i's are the Pauli matrices acting on the A-B space. What is the z component of $\vec{d}$? Draw the vector $\vec{d}$ as a function of momentum in the vicinity of the two Dirac cones, and show that the Dirac cones can indeed be thought of as vortices. What is the winding number of each Dirac cone? Use this to explain the gapping out of the Dirac cones in question iv.

b. Can you think of an additional symmetry breaking that will gap out the Dirac cones?

3. **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. To do so, use the full low energy Hamiltonian, and write it in real space. Then introduce the electromagnetic potential using the minimal substitution. Plot the density of states for positive/negative energies.
    - **b.** What is the degeneracy of each Landau level? Is it different compared to a quadratic dispersion relation?
    - **c.** So far, we have ignored the spin degrees of freedom. Discuss qualitatively what happens when these are included. How does the Zeeman effect change the picture?
4. **Weyl Semimetal** – In class we saw a two-dimensional semi-metallic phase. In this question we will study a tight binding model for a three-dimensional semi-metal. We start with a three-dimensional cubic lattice with two elements, A and B, in each unit cell. Defining $\vec{\psi} = (A(\boldsymbol{k}), \quad B(\boldsymbol{k}))^T$, with $A(\boldsymbol{k}), B(\boldsymbol{k})$ being the annihilation operators in momentum space, we write the Hamiltonian as $H = \sum_{\boldsymbol{k}} \vec{\psi}^{+} h(\boldsymbol{k}) \vec{\psi}$, with $h(\boldsymbol{k}) = t\big(3 - m - cosk_x - cosk_y - cosk_z\big)\sigma_z + t_1 sink_x\, \sigma_x + t_1 sink_y\, \sigma_y$
    Assume throughout this question that the chemical potential is at zero energy.
    - **a.** Write the real-space version of the Hamiltonian.
    - **b.** For which values of m the gap closes. Find the **Exact** locations of these points as a function of m.
    - **c.** Expand the Hamiltonian around the gapless points and write the low energy form of the Hamiltonian.
    - **d.** Focus on the low energy theory you have found. Show that any perturbation acting within a single low energy sector is not capable of opening a gap. Explain (in words) how one can nevertheless open a gap.

e. Add a term of the form $Vsink_z$ to the Bloch Hamiltonian and assume that $V \ll t, t_1$. How does this term alter the low energy theory? What is the shape of the Fermi surface?