Concepts in Condensed Matter Physics: Exercise I

Spring 2018

Due date: 25/04/2018

1. **The spectrum and low energy properties of Graphene**

   Graphene is a material made of a single layer of carbon atoms. This two dimensional system is arranged in a honeycomb lattice, as depicted in figure 1(a). Remember that a honeycomb lattice is actually an hexagonal lattice with a basis of two ions in each unit cell. If a is the distance between nearest neighbors, the primitive lattice vectors can be chosen to be

$$\vec{a}_1 = \tfrac{a}{2}\left(3, \sqrt{3}\right) \quad \vec{a}_2 = \tfrac{a}{2}\left(3, -\sqrt{3}\right), \tag{1}$$

   and the reciprocal-lattice vectors are spanned by

$$\vec{b}_1 = \tfrac{2\pi}{3a}\left(1, \sqrt{3}\right) \quad \vec{b}_2 = \tfrac{2\pi}{3a}\left(1, -\sqrt{3}\right). \tag{2}$$

   The first Brillouin zone is shown in figure 1(b).
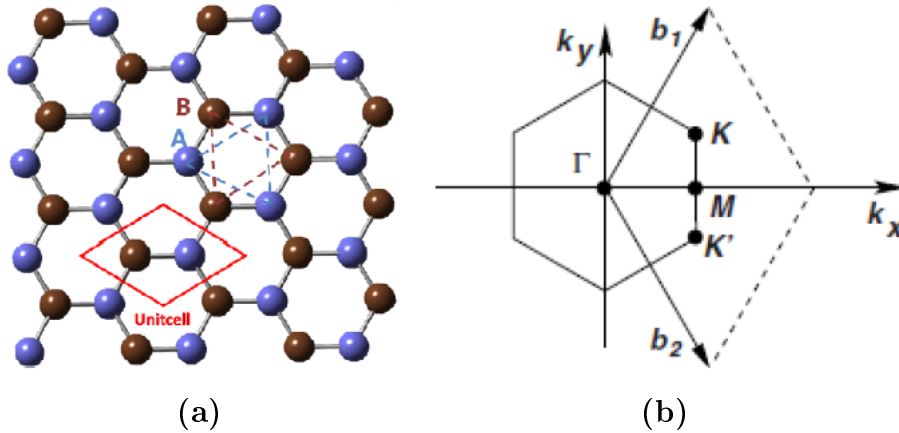

(a)   (b)

Figure 1: (a) Lattice of Graphene. (b) BZ1 of Graphene.

(a) The nearest neighbor hopping tight-binding Hamiltonian of Graphene can be written as

$$H = -t \sum_{\langle \vec{R},\vec{R}'\rangle,\sigma} \left[A^\dagger_{\vec{R},\sigma} B_{\vec{R}',\sigma} + h.c. \right] = -t \sum_{\vec{R},\vec{\delta},\sigma} \left[A^\dagger_{\vec{R},\sigma} B_{\vec{R}+\vec{\delta},\sigma} + h.c. \right] , \tag{3}$$

where the vectors $\vec{\delta}$, connecting the A atoms to their nearest neighbors, are given by

$$\vec{\delta}_1 = \tfrac{a}{2}\left(1,\sqrt{3}\right) \quad \vec{\delta}_2 = \tfrac{a}{2}\left(1,-\sqrt{3}\right) \quad \vec{\delta}_3 = a\left(-1,0\right). \tag{4}$$

Diagonalize the Hamiltonian to find the spectrum and eigenstates of Graphene. Do so by first transforming to k-space and finding the Bloch Hamiltonian $h(\vec{k})$:

$$H = \sum_{\vec{k},\sigma} \vec{\psi}^\dagger_{\vec{k},\sigma} h(\vec{k}) \vec{\psi}_{\vec{k},\sigma} , \tag{5}$$

where $\vec{\psi}_{\vec{k},\sigma} = \left(A_{\vec{k},\sigma}, \ B_{\vec{k},\sigma} \right)^T$. Then diagonalize also the Bloch Hamiltonian. How many bands did you find? Why? Plot the spectrum you obtained as a function of (k_x, k_y) in a 3D plot. Graphene has one electron per atom. Is the spectrum gapless or gapped? Where is the Fermi energy?

(b) The lowest energy excitations above the ground state are the lowest energy states above the Fermi energy. What are the $\vec{k} = (k_x, k_y)$ points of these excitations? *Hint:* You should find six points where the two bands meet (clearly the lowest energy points of the upper band), but some of them will be related by reciprocal lattice vectors. There are only two unique points $\vec{K}$ and $\vec{K}'$.

(c) Find the low energy effective Hamiltonian by expanding the Bloch Hamiltonian in small momentum $\vec{q}$ around $\vec{K}$ and $\vec{K}'$, namely $\vec{k} = \vec{K} + \vec{q}$ with $|q| \ll |K|, |K'|$. Write it using Pauli matrices acting on the A-B space. You should find the 2D massless Dirac Hamiltonian

$$h(\vec{K} + \vec{q}) = \hbar v_F \vec{q} \cdot \vec{\sigma} , \tag{6}$$

and $h(\vec{K}' + \vec{q}) = h^*(\vec{K} + \vec{q})$. Express v_F in terms of the original Hamiltonian parameters. What is the relation between the spectrum of $h(q)$ and that of light? What is the role of v_F?

(d) 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, as we seen in the tutorial, 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:

$$H = -\sum_{\vec{R},\sigma} \sum_a \left[t_a A^\dagger_{\vec{R},\sigma} B_{\vec{R}+\vec{\delta}_a,\sigma} + h.c. \right] \ , \tag{7}$$

where $\vec{\delta}_a$ are the same as in Eq.(4).

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 homogeneous stretching (change the values of 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 $\frac{t_2}{t_1}$ do the Dirac cones gap out?

v. Write the Bloch Hamiltonian in the form $h(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma}$, where the are the Pauli matrices acting on the A-B space. What is the z component of $\vec{d}$? Draw $\vec{d}$ as a function of momentum (k_x, k_y) in the vicinity of the two Dirac cones, and show that the Dirac cones can 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 section iv.

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

3. t/U expansion of the Hubbard Hamiltonian

In class we have derived the low energy effective Hamiltonian of the Hubbard model in the limit $U \gg t$ at half filling using degenerate perturbation theory. To order $\frac{t^2}{U}$ we found the Heisenberg model with $J = \frac{4t^2}{U}$. In this question you will take a different route to expand the Hubbard Hamiltonian in orders of $\frac{t}{U}$ and recover the Heisenberg model once again to the appropriate order at half filling. For simplicity we will use a single index i to label the sites of a d dimensional lattice by some unspecified order. The Hubbard Hamiltonian is:

$$H = T + V = -t \sum_{i,j,\sigma} N_{i,j} c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \ , \tag{8}$$

where $N_{i,j} = 1$ if i and j are nearest neighbors or zero otherwise.

(a) Write the kinetic part, $T = -t \sum_{i,j,\sigma} N_{i,j} c_{i,\sigma}^{\dagger} c_{j,\sigma}$, as a sum over three parts: T_{-1} which decreases the number of double occupied sites by 1, T_0 which keeps the number of doubly occupied sites unchanged, and T_1 which increases the number of doubly occupied sites by 1. Give explicit expressions for the various T_m in terms of the creation and annihilation operators $c^{\dagger}$ and c, the electron number operator n and the hole number operator $h = 1 - n$. *Hint:* multiply T by $(n_{i,\bar{\sigma}} + h_{i,\bar{\sigma}}) = 1$ on the left and by $(n_{j,\bar{\sigma}} + h_{j,\bar{\sigma}}) = 1$ on the right.

(b) Calculate the commutator of the interaction V with the various kinetic terms T_m. What is the meaning of the result you find?

(c) We wish to find a unitary operator S with which to transform the Hamiltonian such that it does not connect states with different numbers of doubly occupied sites. Expand the transformed Hamiltonian $H' = e^{iS} H e^{-iS}$ in a series

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of commutators (the Schrieffer-Wolff transformation) and show that choosing $iS = \frac{1}{U}(T_1 - T_{-1}) + O\left(t^3/U^2\right)$ eliminates T_1 and T_{-1} from $H = V + T_0 + T_1 + T_{-1}]$. What is the resulting H' to this order, $O(t^3/U^2)$? Write it both in terms of V and the various T_m and in terms of the creation and annihilation operators $c^\dagger$ and c, the electron number operator n and the hole number operator $h = 1 - n$.

(d) Now we will specialize to the subspace of states at half filling with no doubly occupied states, i.e., the low energy subspace in the large U limit. Denoting this subspace be L what are $T_0\left|\psi\right\rangle_L$, $T_{-1}\left|\psi\right\rangle_L$ and $V\left|\psi\right\rangle_L$? In light of these results, rewrite the simplified H' when acting on this subspace.

(e) Analyze the form of H' you obtained and rewrite it in terms of the spin operators: $S^z = \left[\frac{1}{2}\left|\uparrow\right\rangle\left\langle\uparrow\right| - \left|\downarrow\right\rangle\left\langle\downarrow\right|\right]$, $S^+ = \left|\uparrow\right\rangle\left\langle\downarrow\right|$ and $S^- = (S^+)^\dagger$, as we did in the tutorial.

It is possible, albeit complicated, to keep constructing iS to higher orders in order to keep eliminating T_1 and T_{-1} to higher orders in H'. At half filling the resulting H' acting on the low energy subspace L will result in a spin model to any order in $\frac{t}{U}$, but the higher order terms in H' will involve more and more spins. Therefore, it is wise to start with the Heisenberg model and analyze various symmetry allowed spin terms on top of it instead.