Concepts in Condensed Matter Physics: Exercise 1a

Spring 2021

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 do 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.

1. 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. 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:

$$H = -\sum_{\vec{R},\sigma} \sum_{a} \left[t_a A^{\dagger}_{\vec{R},\sigma} B_{\vec{R}+\vec{\delta}_a,\sigma} + \text{h.c.} \right] , \tag{1}$$

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

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

(a) 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. Use the form $h(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma}$, where the $\vec{\sigma}$ are the Pauli matrices acting on the A-B space, and find $\vec{d}(\vec{k})$. In what follows you can plot the energy bands numerically.

(b) What happens to the Dirac cones in homogeneous stretching (change the values of the t's but keep them equal)?

(c) How are the two Dirac points and cones affected in the following two different cases: (i) $t_1 = t_3 > t_2$, and (ii) $t_1 = t_3 < t_2$? For what values of $r \equiv \frac{t_2}{t_1}$ do the Dirac cones gap out? Plot the band structure of the Bloch Hamiltonian for several representative values of r leading up to r^* where the cones gap out. Plot the phase of the pseudo-spin wave-function as a function of $\vec{k}$ for these values of r in the vicinity of the Dirac points. (Similar to what you saw in class for non-stretched case.) Try explaining what happens to the Dirac cones in terms of vortices in k-space as r is modified.

(d) For the non-stretched case, we found the Hamiltonian

$$\tilde{H} = \hbar v_F \left(k_x \sigma_x + \tau_z k_y \sigma_y \right) , \tag{3}$$

with $\tau_z = \pm 1$ labeling the valley degree of freedom. How does Eq. (3) change when the graphene is stretched? (You may assume $r \ll r^*$.) Compare this to the coupling of the Dirac fermions to the electromagnetic gauge field $p_\mu \to p_\mu - qA_\mu$.

2. What happens when one introduces a term proportional to σ_z (for example $d_z =$ const.) to $h(\vec{k})$? What is the physical meaning of such a term, and how does it manifest in the microscopic tight-binding Hamiltonian? What symmetry of Graphene does it break?