8.513 Problem Set # 9

Problems:

1. **Gapless chiral edge model of a Chern insulator** (20 pts)

   The electrons in graphene near one of the Dirac point, the K-point in BZ, are described by a Hamiltonian (in real space)

   $$H_K = -\mathrm{i}v\hbar(\sigma^y\partial_x + \sigma^x\partial_y) \tag{1}$$

   The Hamiltonian acts on two-component wave function $\Psi(\boldsymbol{x}) = \begin{pmatrix}\psi_1(\boldsymbol{x})\\ \psi_2(\boldsymbol{x})\end{pmatrix}$. The energy eigenfunction is given by

   $$H_K\Psi = -\mathrm{i}v\hbar(\sigma^y\partial_x + \sigma^x\partial_y)\Psi(\boldsymbol{x}) = \epsilon\Psi(\boldsymbol{x}). \tag{2}$$

   One the other hand, the electrons near the other Dirac point, the K'-point in BZ, are described by a Hamiltonian (in real space)

   $$H_{K'} = -\mathrm{i}v\hbar(\sigma^y\partial_x - \sigma^x\partial_y) \tag{3}$$

   Note the different handness.

   If the two sites in the unit cell of graphene have different potentials V and $-V$ (as in Boron Nitride), the Dirac fermion near K and K' will be described by

   $$\begin{aligned} H_K^{\text{trivial}} &= -\mathrm{i}v\hbar(\sigma^y\partial_x + \sigma^x\partial_y) + V\sigma^z \\ H_{K'}^{\text{trivial}} &= -\mathrm{i}v\hbar(\sigma^y\partial_x - \sigma^x\partial_y) + V\sigma^z \end{aligned} \tag{4}$$

   Now, the conduction band and valence band no longer tough at the K and K' point, and the system becomes a trivial insulator.

   However, in the Haldane model, the Dirac fermion near K and K' will be described by

   $$\begin{aligned} H_K^{\text{Chern}} &= -\mathrm{i}v\hbar(\sigma^y\partial_x + \sigma^x\partial_y) + \sqrt{3}t'\sigma^z \\ H_{K'}^{\text{Chern}} &= -\mathrm{i}v\hbar(\sigma^y\partial_x - \sigma^x\partial_y) - \sqrt{3}t'\sigma^z \end{aligned} \tag{5}$$

   Like the $V\sigma^z$-terms above, the $t'\sigma^z$-terms also open an energy gap and the conduction band and valence band no longer tough at the K and K' point. But in this case, the system becomes a Chern insulator.

   We see that the difference between the trivial insulator and the Chern insulator is that the "mass" term (*ie* the σ^z term) of the Dirac fermions at K and K' point have different signs. For the trivial insulator, the sign of the mass term is $+, +$. For the Chern insulator, the sign of the mass term is $+, -$. In other words, if we change the sign of the Dirac fermion mass term at K' from $+$ to $-$, we will change a trivial insulator to a Chern insulator.

   In this problem, we will consider a domain wall between a trivial insulator and a Chern insulator by changing the mass term (the σ^z term) for positive mass to negative mass for the Dirac fermions at K'-point. By solving the Dirac equation with spatial dependent mass term, we can derive the gapless chiral edge modes on the domain wall between a trivial insulator and a Chern insulator.

Let us consider the Hamiltonian for the Dirac fermions near the K'-point with a spatial dependent mass $m(y)$:

$$H_{K'} = -\mathrm{i}v\hbar(\sigma^z\partial_x - \sigma^y\partial_y) + m(y)\sigma^x. \tag{6}$$

To simply the later calculations, we have made a cyclic shift to the σ-matrix: $\sigma^x \to \sigma^y$, $\sigma^y \to \sigma^z$, $\sigma^z \to \sigma^x$. For simplicity, we choose $m(y) = y$ and $v\hbar = 1$

$$H_{K'} = -\mathrm{i}(\sigma^z\partial_x - \sigma^y\partial_y) + y\sigma^x. \tag{7}$$

The $y > 0$ region corresponds to a trivial insulator and the $y < 0$ region corresponds to a Chern insulator. The eigenstates of $H_{K'}$ near the zero energy will correspond to the gapless edge states (assuming the chemical potential, *ie* the Fermi energy, is chosen to be $\mu = E_F = 0$). (Note that near K-point, H_K has no eigenstates near the zero energy due to the gap, and hence does not contribute to gapless edge modes).

Now we look for the eigenstate of $H_{K'}$, $\Psi(x, y)$, with energy ϵ

$$[-\mathrm{i}(\sigma^z\partial_x - \sigma^y\partial_y) + y\sigma^x]\Psi(x,y) = \begin{pmatrix} -\mathrm{i}\partial_x & \partial_y + y \\ -\partial_y + y & \mathrm{i}\partial_x \end{pmatrix} \Psi(x,y) = \epsilon\Psi(x,y). \tag{8}$$

Due to the translation symmetry in the x-direction, the eigenstate has a form

$$\Psi(x,y) = \mathrm{e}^{\mathrm{i}kx}\Psi_k(y) \tag{9}$$

where the two-component wave function $\Psi_k(y)$ only depends on y.

(a) Show that, for each fixed k, there are two eigenfunctions of the form

$$\Psi(x,y) = \mathrm{e}^{\mathrm{i}kx}\Psi_k(y) = \mathrm{e}^{\mathrm{i}kx}\begin{pmatrix} \#\mathrm{e}^{\alpha_1 y^2} \\ 0 \end{pmatrix}$$
$$\Psi(x,y) = \mathrm{e}^{\mathrm{i}kx}\Psi_k(y) = \mathrm{e}^{\mathrm{i}kx}\begin{pmatrix} 0 \\ \#\mathrm{e}^{\alpha_2 y^2} \end{pmatrix} \tag{10}$$

Find the eigenfunctions and show that one of them is not normalizable and should be dropped.

(b) Find the energy eigenvalue $\epsilon(k)$ as a function of k. You will see that there is only one chiral mode near Fermi energy $E_F = 0$.
(If we did not drop the eigenfunctions that are not normalizable, we would have two gapless modes, one right-mover and one left-mover.)

(c) The Hamiltonian (7) also has other bands. Describe and sketch the dispersion relations of those bands.

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