8.231 Physics of Solids I — Fall 2017
Recitation 6

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1 Dirac Fermion as $k \cdot p$ Theory

Recall the tight-binding Hamiltonian of graphene:

$$H(\mathbf{k}) = \begin{pmatrix} 0 & -t\sum_{i=1}^{3} e^{-i\mathbf{k}\cdot\mathbf{d}_i} \\ -t\sum_{i=1}^{3} e^{i\mathbf{k}\cdot\mathbf{d}_i} & 0 \end{pmatrix}, \tag{1}$$

where we have set the atomic energy $\mathcal{E} = 0$ for simplicity. Around K/K' point the Brillouin zone, the Hamiltonian can be expanded as

$$H(\mathbf{q}) = vq_x\sigma_x + vq_y\sigma_y, \tag{2}$$

where $\mathbf{q} \equiv \mathbf{k} - \mathbf{K}/\mathbf{K}'$. The Hamiltonians of form Eq. (2) are often referred to as $k \cdot p$ Hamiltonians, where k refers to a vector of momentum p refers to a vector operators (here they are Pauli matrices). $k \cdot p$ Hamiltonians are useful to study the low energy properties of solids.

The Hamiltonian of two-dimensional Dirac fermion can be generally written as

$$H(\mathbf{k}) = vk_x\sigma_x + vk_y\sigma_y + m\sigma_z. \tag{3}$$

In graphene, the Dirac fermion is massless $m = 0$. In boron nitride, the Dirac fermion has mass which is half of the band gap. In the following, we will set $v = 1$ for simplicity.

The energy dispersion of Dirac fermion is

$$E_{\pm}(\mathbf{k}) = \pm\sqrt{k_x^2 + k_y^2 + m^2}. \tag{4}$$

The (unnormalized) energy eigenstates are

$$\psi_{\pm}(\mathbf{k}) = \begin{pmatrix} m \pm \sqrt{k_x^2 + k_y^2 + m^2} \\ k_x + ik_y \end{pmatrix}. \tag{5}$$

Note that the gapped band structure when $m > 0$ cannot be continuously deformed to that when $m < 0$ without closing the band gap. It is usually said that these two band structures are in different phases.

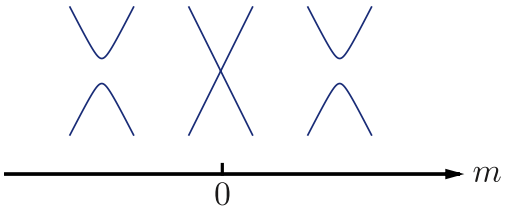

Figure 1: Topological phase diagram of the two-dimensional Dirac fermion.

2 Edge State from Domain Wall Problem

Due to the topologically in-equivalence of the two phases, there will be a localized edge state in the boundary of two Dirac fermions of opposite masses.

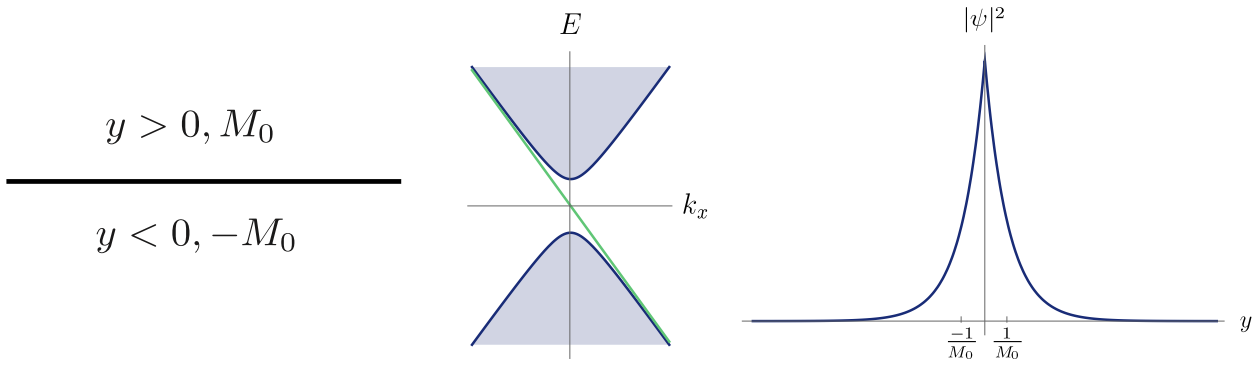

Figure 2: Left: Geometry of the domain wall problem; Middle: Dispersion of the bulk band (blue) and the edge state (green); Right: Localized wavefunction probability distribution.

Consider a domain wall problem of two semi-infinite planes separated by $y = 0$. The Hamiltonians within each domain are Dirac fermions, whose fermion masses are of different signs. Formally, the Hamiltonian can be written as

$$H = -i\partial_x\sigma_x - i\partial_y\sigma_y + m(y)\sigma_z, \tag{6}$$

where

$$m(y) = M_0\theta(y) - M_0\theta(-y). \tag{7}$$

$\theta(y)$ is the step function. We have set $\hbar = 1$ for simplicity. Without loss of generality we will also $M_0 > 0$ in the following.

First notice that k_x is still a good quantum number. The energy eigenstates should be of the form $\psi(x, y) = e^{ikx}\psi_k(y)$. The eigenvalue problem then becomes

$$\left[k_x\sigma_x - i\partial_y\sigma_y + m(y)\sigma_z\right]\psi_k(y) = E\psi_k(y), \tag{8}$$

which can be more explicitly written as

$$\begin{pmatrix} m(y) & k_x - i\partial_y \\ k_x + i\partial_y & -m(y) \end{pmatrix}\begin{pmatrix}\psi_{k,1}\\ \psi_{k,2}\end{pmatrix} = E\begin{pmatrix}\psi_{k,1}\\ \psi_{k,2}\end{pmatrix}. \tag{9}$$

Within each domain, Eq. (9) is the same as the Dirac equation. So the solution is also of the same form as Eq. (5), with k_y to be determined by the boundary condition. In this way, we can write down the ansatz for Eq. (9)

$$\psi_k(y) = c_1\begin{pmatrix} M_0 \pm \sqrt{k_x^2 - \kappa_1^2 + M_0^2} \\ k_x - \kappa_1 \end{pmatrix} e^{-\kappa_1 y}\theta(y) + c_2\begin{pmatrix} -M_0 \pm \sqrt{k_x^2 - \kappa_2^2 + M_0^2} \\ k_x + \kappa_2 \end{pmatrix} e^{\kappa_2 y}\theta(-y), \tag{10}$$

where the $\kappa_1 \equiv -ik_{y,1}$ and $\kappa_2 \equiv ik_{y,2}$. c_1 and c_2 are normalization factors. In order for the wavefunction to be normalizable: $\kappa_1, \kappa_2 > 0$. In order for the two solutions in the separate domains to give the same energy eigenvalue E, we have $\sqrt{k_x^2 - \kappa_1^2 + M_0^2} = \sqrt{k_x^2 - \kappa_2^2 + M_0^2}$. This implies $\kappa_1^2 = \kappa_2^2 \equiv \kappa^2$. Finally, the wavefunction must be continuous along $y = 0$, thus

$$\frac{M_0 \pm \sqrt{k_x^2 - \kappa^2 + M_0^2}}{k_x - \kappa} = \frac{-M_0 \pm \sqrt{k_x^2 - \kappa^2 + M_0^2}}{k_x + \kappa}. \tag{11}$$

It is not hard to verify the solution is $\kappa = M_0$. When $k_x > 0$ ($k_x < 0$), the equation holds by taking the minus (plus) sign. The energy dispersion of this state is $E = -k_x$. The probability density of this state decays exponentially away from the edge, thus the state is a localized edge state. The localization length is $\xi = 1/\kappa = 1/M_0$.

For a general functional form of $m(y)$, the domain wall problem can still be solved by replacing $e^{\pm\kappa y}$ to $e^{-\int_0^y m(y')dy'}$.

Experimentally, one domain is continuously connected to the vacuum, while another domain represents the topologically non-trivial insulator. The edge state will be found at the surface of the material.