1 Dirac Fermion as $k \cdot p$ Theory

Recall the tight-binding Hamiltonian of graphene:

$$H(k) = \begin{pmatrix} 0 & -t \sum_{i=1}^{3} e^{ikd_i} \\ -t \sum_{i=1}^{3} e^{-ikd_i} & 0 \end{pmatrix},$$

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

$$H(q) = vqx_x + vqy\sigma_y,$$

where $q \equiv k - K/K'$. The Hamiltonians of form Eq. (1) are often referred to as $k \cdot p$ Hamiltonians, where $k$ refers to a vector of momentum and $p$ 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

$$H(k) = vk_x\sigma_x + vk_y\sigma_y + m\sigma_z.$$

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

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

The (unnormalized) energy eigenstates are

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

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.
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.

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

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

where

$$m(y) = M_0 \theta(y) - M_0 \theta(-y).$$

$\theta(y)$ 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

$$[k_x \sigma_x - i\partial_y \sigma_y + m(y)\sigma_z] \psi_k(y) = E\psi_k(y),$$

which can be more explicitly written as

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

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. (11)

$$\psi_k(y) = c_1 \left( \frac{M_0 \pm \sqrt{k_x^2 - \kappa_1^2 + M_0^2}}{k_x - \kappa_1} \right) e^{-\kappa_1 y} \theta(y) + c_2 \left( -\frac{M_0 \pm \sqrt{k_x^2 - \kappa_2^2 + M_0^2}}{k_x + \kappa_2} \right) e^{\kappa_2 y} \theta(-y),$$

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

$$\frac{M_0 \pm \sqrt{k_x^2 - \kappa^2 + M_0^2}}{k_x - \kappa} = -\frac{M_0 \pm \sqrt{k_x^2 - \kappa^2 + M_0^2}}{k_x + \kappa}.$$
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 $e^{\pm k_y}$ to $e^{-\int_{y_0}^{y} m(y') dy'}$.

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.