Chapter 2
Starting from the Dirac Equation

Abstract The Dirac equation is the key to understanding topological insulators and superconductors. A quadratic correction to the equation makes it topologically distinct. The solution of the bound states near the boundary reflects the topology of the system's band structure.

2.1 Dirac Equation

In 1928, Paul A.M. Dirac wrote an equation for a relativistic quantum mechanical wave function that describes an elementary spin-$\frac{1}{2}$ particle [1, 2],

$$H = c\mathbf{p} \cdot \alpha + mc^2\beta, \tag{2.1}$$

where m is the rest mass of a particle and c is the speed of light. α_i and β are known as the Dirac matrices that satisfy the relations

$$\alpha_i^2 = \beta^2 = 1, \tag{2.2}$$

$$\alpha_i \alpha_j = -\alpha_j \alpha_i, \tag{2.3}$$

$$\alpha_i \beta = -\beta \alpha_i. \tag{2.4}$$

Here a_i and β are not simple complex numbers. The anticommutation relation means that they can obey a Clifford algebra and must be expressed in a matrix form. In one- and two-dimensional spatial space, they are at least 2×2 matrices. The Pauli matrices σ_i ($i = x, y, z$) satisfy all these relations,

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}, \tag{2.5}$$

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where

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.6}$$

Thus, in one dimension, the two Dirac matrices α_x and β are any two of the three Pauli matrices, for example,

$$\alpha_x = \sigma_x, \beta = \sigma_z. \tag{2.7}$$

In two dimensions, the three Dirac matrices are the Pauli matrices,

$$\alpha_x = \sigma_x, \alpha_y = \sigma_y, \beta = \sigma_z. \tag{2.8}$$

In three dimensions, we cannot find more than three 2×2 matrices that satisfy the anticommutation relations. Thus, the four Dirac matrices are at least 4-dimensional, and can be expressed in terms of the Pauli matrices

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \equiv \sigma_x \otimes \sigma_i, \tag{2.9}$$

$$\beta = \begin{pmatrix} \sigma_0 & 0 \\ 0 & -\sigma_0 \end{pmatrix} \equiv \sigma_z \otimes \sigma_0, \tag{2.10}$$

where σ_0 is a 2×2 identity matrix.

From this equation, the relativistic energy-momentum relation will be automatically the solution of the following equation:

$$E^2 = m^2c^4 + p^2c^2. \tag{2.11}$$

In three dimensions, there are two solutions for positive energy E_+ and two solutions for negative energy E_-,

$$E_\pm = \pm\sqrt{m^2c^4 + p^2c^2}. \tag{2.12}$$

This equation can be used to describe the motion of an electron with spin: the two solutions of the positive energy correspond the two states of an electron, spin-up and down, and the two solutions of the negative energy correspond to the two states of an positron with spin-up and down. The energy gap between these two particles is $2mc^2 (\approx 1.0\,\mathrm{MeV})$.

This equation requires the existence of an antiparticle, i.e., a particle with negative energy or mass, and predates the discovery of positrons, the antiparticles of an electron. It is one of the main achievements of modern theoretical physics. Dirac proposed that the negative energy states are fully filled, and the Pauli exclusion principle prevents a particle transiting into these occupied states. The normal state of the vacuum then consists of an infinite density of negative energy states. The state of a single electron means that all the states of negative energies are filled, and only one state of positive energy is filled. It is assumed that any deviation from the norm produced by employing one or more of the negative energy states can be observed. The absence of a negative charged electron that has a negative mass and kinetic energy would then manifest itself as a positively charged particle that has an equal positive mass and positive energy. In this way, a hole or positron can be formulated. Unlike the Schrödinger equation for a single particle, the Dirac theory, in principle, is a many-body theory. This has been discussed in many textbooks on relativistic quantum mechanics [2].

Under the transformation of mass $m \to -m$, it is found that the equation remains invariant if we replace $\beta \to -\beta$, which satisfies all of the mutual anticommutation relations for α_i and β in (2.4). This reflects the symmetry between the positive and negative energy particles in the Dirac equation: there is no topological distinction between particles with positive and negative masses.

2.2 Solutions of Bound States

2.2.1 Jackiw-Rebbi Solution in One Dimension

A possible relation between the Dirac equation and the topological insulator is revealed by a solution of the bound state at the interface between the regions of positive and negative masses. We start with

$$h(x) = -iv\hbar\partial_x\sigma_x + m(x)v^2\sigma_z \tag{2.13}$$

and

$$m(x) = \begin{cases} -m_1 & \text{if} \quad x < 0 \\ +m_2 & \text{otherwise} \end{cases} \tag{2.14}$$

(and m_1 and $m_2 > 0$). We use an effective velocity v to replace the speed of light c when the Dirac equation is applied to solids. The eigenvalue equation has the form

$$\begin{pmatrix} m(x)v^2 & -iv\hbar\partial_x \\ -iv\hbar\partial_x & -m(x)v^2 \end{pmatrix} \begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix} = E \begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix}. \tag{2.15}$$

For either $x < 0$ or $x > 0$, the equation is a second-order ordinary differential equation. We can solve the equation at $x < 0$ and $x > 0$ separately. The solution of the wave function should be continuous at $x = 0$. In order to have a solution of a bound state near the junction, we take the Dirichlet boundary condition that the wave function must vanish at $x = \pm\infty$. For $x > 0$, we set the trial wave function as

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix} = \begin{pmatrix} \varphi_1^+ \\ \varphi_2^+ \end{pmatrix} e^{-\lambda_+ x}. \tag{2.16}$$

Then the secular equation gives

$$\det \begin{pmatrix} m_2 v^2 - E & i v \hbar \lambda_+ \\ i v \hbar \lambda_+ & -m_2 v^2 - E \end{pmatrix} = 0. \tag{2.17}$$

The solution to this equation is $\lambda_+ = \pm\sqrt{m_2^2 v^4 - E^2}/v\hbar$.

The solutions λ can be either real or purely imaginary. For $m_2^2 v^4 < E^2$ the solutions are purely imaginary, and the corresponding wave functions spread over the whole space. These are the extended states or the bulk states, which we are not interested in here. For $m_2^2 v^4 > E^2$ the solutions are real, and we choose a positive λ_+ to satisfy the boundary condition at $x \to +\infty$. The two components in the wave function satisfy

$$\varphi_1^+ = -\frac{i v \hbar \lambda_+}{m_2 v^2 - E} \varphi_2^+. \tag{2.18}$$

Similarly, for $x < 0$, we have

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix} = \begin{pmatrix} \varphi_1^- \\ \varphi_2^- \end{pmatrix} e^{+\lambda_- x} \tag{2.19}$$

with $\lambda_- = \sqrt{m_1^2 v^4 - E^2}/v\hbar$, and

$$\varphi_1^- = -\frac{i v \hbar \lambda_-}{m_1 v^2 + E} \varphi_2^-. \tag{2.20}$$

At $x = 0$, the continuity condition for the wave function requires

$$\begin{pmatrix} \varphi_1^+ \\ \varphi_2^+ \end{pmatrix} = \begin{pmatrix} \varphi_1^- \\ \varphi_2^- \end{pmatrix}. \tag{2.21}$$

From this equation, it follows that

$$\frac{-\sqrt{m_2^2 v^4 - E^2}}{m_2 v^2 - E} = \frac{\sqrt{m_1^2 v^4 - E^2}}{-m_1 v^2 - E}. \tag{2.22}$$

Thus, there exists a solution of zero energy, $E = 0$, and the corresponding wave function is

$$\Psi(x) = \sqrt{\frac{v}{\hbar} \frac{m_1 m_2}{m_1 + m_2}} \begin{pmatrix} i \\ 1 \end{pmatrix} e^{-|m(x) v x|/\hbar}. \tag{2.23}$$

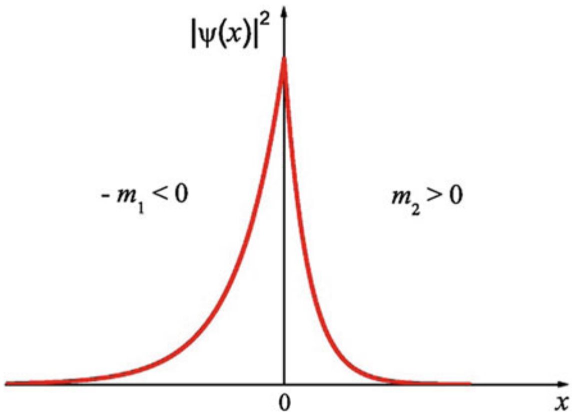

Fig. 2.1 Probability density $|\Psi(x)|^2$ of the solution as a function of its position in (2.23)

The solution is dominantly distributed near the interface or domain wall at $x = 0$ and decays exponentially away from the point $x = 0$ as shown in Fig. 2.1. The solution of $m_1 = m_2$ was first obtained by Jackiw and Rebbi, and is the mathematical basis for the existence of topological excitations or solitons in one-dimensional systems [3]. The spatial distribution of the wave function are determined by the characteristic scales $\xi_{1,2} = \lambda_{\pm}^{-1} = \hbar / \left| m_{1,2} v \right|$. The solution exists even when $m_2 \to +\infty$. In this case, $\Psi(x) \to 0$ for $x > 0$. However, we have to point out that the wave function is not continuous at the interface, $x = 0$. If we regard the vacuum as a system with an infinite positive mass, a system with a negative mass with an open boundary condition possesses a bound state near the boundary if the continuity condition is relaxed to the wave function. This result leads to some popular impression of the formation of the edge and surface states in topological insulators.

With regards to the stability of the zero mode solution, we may find a general solution of zero energy for a distribution of mass $m(x)$ that changes from a negative to positive mass at two ends. Consider the solution of $E = 0$ for (2.13). The eigenvalue equation is reduced to

$$\left[-iv\hbar\partial_x\sigma_x + m(x)v^2\sigma_z\right]\varphi(x) = 0. \tag{2.24}$$

Multiplying σ_x from the left hand side, one obtains

$$\partial_x\varphi(x) = -\frac{m(x)v}{\hbar}\sigma_y\varphi(x). \tag{2.25}$$

Thus, the wave function should be the eigenstate of σ_y,

$$\sigma_y\varphi_\eta(x) = \eta\varphi_\eta(x) \tag{2.26}$$

with

$$\varphi_{\pm} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm i \end{pmatrix}\varphi(x).$$

The wave function has the form

$$\varphi_{\eta}(x) \propto \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \eta i \end{pmatrix}\exp\left[-\int^{x}\eta\frac{m(x)v}{\hbar}dx'\right]. \tag{2.27}$$

For $x \to \pm\infty$, $\varphi(x) \propto \exp\left[-\left|m(\pm\infty)vx\right|/\hbar\right]$, and the sign η is determined by the signs of $m(\pm\infty)$. If $m(+\infty)$ and $m(-\infty)$ differ by a sign as a domain wall, there always exists a zero energy solution near a domain wall of the mass distribution $m(x)$. Therefore this solution is quite robust against the mass distribution $m(x)$.

2.2.2 Two Dimensions

In two dimensions (with $p_z = 0$), we consider a system with an interface at $x = 0$, $m(x) = -m_1$ for $x < 0$, and m_2 for $x > 0$. $p_y = \hbar k_y$ is a good quantum number. We have two solutions which the wave functions dominantly distribute around the interface: one solution has the form

$$\Psi_{+}(x, k_y) = \sqrt{\frac{v}{h}\frac{m_1 m_2}{m_1 + m_2}}\begin{pmatrix} i \\ 0 \\ 0 \\ 1 \end{pmatrix} e^{-|m(x)vx|/\hbar + ik_y y} \tag{2.28}$$

with the dispersion $\epsilon_{k,+} = v\hbar k_y$ and the other has the form

$$\Psi_{-}(x, k_y) = \sqrt{\frac{v}{h}\frac{m_1 m_2}{m_1 + m_2}}\begin{pmatrix} 0 \\ i \\ 1 \\ 0 \end{pmatrix} e^{-|m(x)vx|/\hbar + ik_y y} \tag{2.29}$$

with the dispersion $\epsilon_{k,-} = -v\hbar k_y$. We can check these two solutions in the following way. The Dirac equation can be divided into two parts,

$$H = [m(x)v^2\beta + vp_x\alpha_x] + vp_y\alpha_y. \tag{2.30}$$

From the one-dimensional solution one has

$$(m(x)v^2\beta + vp_x\alpha_x)\Psi_{\pm} = 0 \tag{2.31}$$

and

$$vp_y\alpha_y\Psi_\pm = \pm vp_y\Psi_\pm. \tag{2.32}$$

From the dispersions of the two states, the effective velocities of the electrons in the states are

$$v_\pm = \frac{\partial\epsilon_{k,\pm}}{\hbar\partial k} = \pm v. \tag{2.33}$$

Therefore, each state carries a current along the interface, but the electrons with different spins move in opposite directions. The current density decays exponentially away from the interface. As the system has the time reversal symmetry, the two states are time reversal counterpart of each other, constituting a pair of helical edge (or bound) states at the interface. Furthermore, the Dirac equation of $p_z = 0$ can be reduced to two independent sets of equations

$$h(x) = vp_x\sigma_x \pm vp_y\sigma_y + m(x)v^2\sigma_z \tag{2.34}$$

for different spins. Thus, it is clear why two bound states have opposite velocities.

2.2.3 Three and Higher Dimensions

In three and higher dimensions, bound states always exist at the interface of the system with positive and negative masses. Even when all other components of the momentum in the interface are good quantum numbers, there is always a solution for zero momentum, as in the one-dimensional case. We can use these solutions to derive the ones of non-zero momenta in higher dimensions.

2.3 Why not the Dirac Equation?

From the Dirac equation, we know there is a solution of bound states at the interface between two media with positive and negative masses or energy gaps. These solutions are quite robust against the roughness of the interface or other factors. If we assume that the vacuum is an insulator with an infinitely large and positive mass or energy gap, then the system with a negative mass should have bound states around the open boundary only if the contiuity condition of the wave function is relaxed. This is very close to the definition of topological insulators. However, because of the symmetry in the Dirac equation with positive and negative masses, there is no topological distinction between these two systems after a unitary transformation. We cannot determine which one is topologically trivial or non-trivial simply from the sign of the mass or energy gap. If we use the Dirac equation to describe a topological insulating phase, we have to introduce or assign an additional "vacuum" as a benchmark. Thus, we think this additional condition is unnecessary as the existence of the bound state should be a physical and intrinsic consequence of the band structure in topological insulators. Therefore we conclude that the Dirac equation in (2.1) itself may not be a "suitable" candidate to describe the topology of quantum matters.

2.4 Quadratic Correction to the Dirac Equation

To explore a possible description of a the topological insulator, we introduce a quadratic correction $-Bp^2$ in momentum $\mathbf{p}$ to the band gap or rest-mass term in the Dirac equation [4],

$$H = v\mathbf{p} \cdot \alpha + \left(mv^2 - B\mathbf{p}^2\right) \beta, \tag{2.35}$$

where mv^2 is the band gap of the particle and m and v have dimensions of mass and speed, respectively. B^{-1} also has the dimension of mass. The quadratic term breaks the symmetry between the mass m and $-m$ in the Dirac equation, and makes this equation topologically distinct from the original Dirac equation in (2.1).

To illustrate this, we plot the spin distribution of the ground state in momentum space as shown in Fig. 2.2. At $p = 0$, the spin orientation is determined by $mv^2\beta$ or the sign of mass m, but for a large p, it is determined dominantly by $-B\mathbf{p}^2\beta$ or the sign of B. If the dimensionless parameter $mB > 0$, when p increases along one direction, say the x-direction, the spin will rotate from the z-direction to the x-direction of $\mathbf{p}$ at $p_c^2 = mv^2/B$, and then eventually to the opposite z-direction for a larger $\mathbf{p}$. This consists of two so-called merons in momentum space, which is named

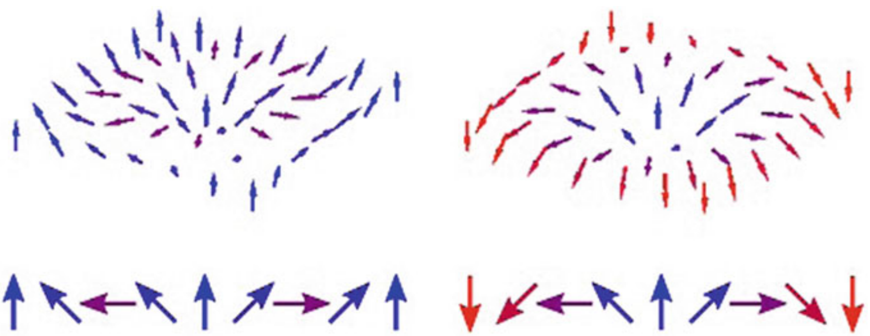

Fig. 2.2 Spin orientation in momentum space. *Left* ($mB < 0$) the spins at $p = 0$ and $p = +\infty$ are parallel, which is topologically trivial. *Left bottom* spin orientation along the p_x-axis. *Right* ($mB > 0$) the spins at $p = 0$ and $p = +\infty$ are anti-parallel, which is topologically non-trivial. *Right bottom* spin orientation along the p_x-axis

skymion. For $mB < 0$, when p increases, the spin will rotate from the z-direction to the direction of p, and then flips back to the initial z-direction. The question of whether the spin points in the same direction at $p = 0$ and $+\infty$ determines whether the equation is topologically distinct in the case of $mB > 0$ and $mB < 0$.

2.5 Bound State Solutions of the Modified Dirac Equation

2.5.1 *One Dimension: End States*

Let us start with a one-dimensional case. In this case, the 4×4 (2.35) can be decoupled into two independent sets of 2×2 equations,

$$h(x) = vp_x\sigma_x + \left(mv^2 - Bp_x^2\right)\sigma_z. \tag{2.36}$$

For a semi-infinite chain with $x \geq 0$, we consider an open boundary condition at $x = 0$. It is required that the wave function vanishes at the boundary, i.e., the Dirichlet boundary condition. Usually, we have a series of solutions of extended states, which wave functions spread throughout the whole space. In this section, we focus on the solution of the bound state near the boundary. To find the solution of zero energy, we have

$$\left[vp_x\sigma_x + \left(mv^2 - Bp_x^2\right)\sigma_z\right]\varphi(x) = 0. \tag{2.37}$$

Multiplying σ_x from the left hand side, one obtains

$$\partial_x\varphi(x) = -\frac{1}{v\hbar}\left(mv^2 + B\hbar^2\partial_x^2\right)\sigma_y\varphi(x). \tag{2.38}$$

If $\varphi(x)$ is an eigen function of σ_y, take $\varphi(x) = \chi_\eta\phi(x)$ with $\sigma_y\chi_\eta = \eta\chi_\eta$ $(\eta = \pm 1)$. Then, the differential equation is reduced to the second-order ordinary differential equation,

$$\partial_x\phi(x) = -\frac{\eta}{v\hbar}\left(mv^2 + B\hbar^2\partial_x^2\right)\phi(x). \tag{2.39}$$

Taking the trial wave function $\phi(x) \propto e^{-\lambda x}$, one obtains the secular equation

$$B\hbar^2\lambda^2 - \eta v\hbar\lambda + mv^2 = 0. \tag{2.40}$$

The two roots satisfy the relation $\lambda_+ + \lambda_- = \eta v\hbar/B$ and $\lambda_+\lambda_- = mv^2/B\hbar^2$. To have a bound state solution, it is required that the wave function vanishes at $x = 0$ and $x = +\infty$,

$$\varphi(x = 0) = \varphi(x = +\infty) = 0. \tag{2.41}$$

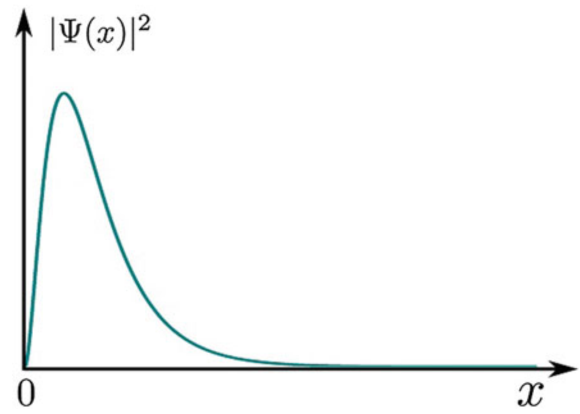

Fig. 2.3 Schematic of the probability density $|\Psi(x)|^2$ of the end state solution as a function of its position in (2.42)

The two roots should be positive and only one of χ_η satisfy the boundary condition for a bound state, $\eta = sgn(B)$ (without loss of generality, we assume that v is always positive). In the condition of $mB > 0$, there exists a solution of the bound state with zero energy

$$\varphi_\eta(x) = \frac{C}{\sqrt{2}} \begin{pmatrix} sgn(B) \\ i \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-}), \tag{2.42}$$

where $\xi_\pm^{-1} = \frac{v}{2|B|\hbar}\left(1 \pm \sqrt{1-4mB}\right)$ and C is the normalization constant. The main feature of this solution is that the wave function distributes dominantly near the boundary, and decays exponentially away from one end as shown in Fig. 2.3. The two parameters ξ_+ and ξ_- decide the spatial distribution of the wave function. These are two important length scales, which characterize the end states. When $B \to 0$, $\xi_+ \to |B|\,\hbar/v$ and $\xi_- = \hbar/mv$, i.e., ξ_+ approaches to zero, and ξ_- becomes a finite constant that is determined by the energy gap mv^2. If we relax the constraint of the vanishing wave function at the boundary, the solution exists even if $B = 0$. In this way, we go back to the conventional Dirac equation. In this sense, the two equations reach the same conclusion. When $m \to 0$, $\xi_- = \hbar/mv \to +\infty$ and the state evolves into a bulk state. Thus, the end states disappear and a topological quantum phase transition occurs at $m = 0$.

In the four-component form to (2.35), two degenerate solutions have the form,

$$\Psi_1 = \frac{C}{\sqrt{2}} \begin{pmatrix} sgn(B) \\ 0 \\ 0 \\ i \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-}) \tag{2.43}$$

and

$$\Psi_2 = \frac{C}{\sqrt{2}} \begin{pmatrix} 0 \\ sgn(B) \\ i \\ 0 \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-}). \tag{2.44}$$

We shall see that these two solutions can be used to derive effective Hamiltonians for higher dimensional systems.

The role of this solution cannot be underestimated in the theory of topological insulators. We will see that all solutions of the edge or surface states, and topological excitations are closely related to this solution.

2.5.2 Two Dimensions: Helical Edge States

In two dimensions, the equation can also be decoupled into two independent equations

$$h_{\pm} = vp_x\sigma_x \pm vp_y\sigma_y + \left(mv^2 - Bp^2\right)\sigma_z. \tag{2.45}$$

These two equations break the "time" reversal symmetry under the transformation of $\sigma_i \to -\sigma_i$ and $p_i \to -p_i$, although the original four-component equation is time reversal invariant.

We consider a semi-infinite plane with the boundary at $x = 0$. $p_y = \hbar k_y$ is a good quantum number. At $k_y = 0$, the two-dimensional equation has the identical form as the one-dimensional equation. The x dependent part of the solution has the identical form as in the one dimension. Thus, we use the two one-dimensional solutions $\{\Psi_1, \Psi_2\}$ in (2.43) and (2.44) as the basis of the two-dimensional solutions. The y dependent part $\Delta H_{2D} = vp_y\alpha_y - Bp_y^2\beta$ is regarded as the perturbation to the one-dimensional Hamiltonian. In this way, we have a one-dimensional effective model for the helical edge states

$$H_{eff} = (\langle\Psi_1|\,, \langle\Psi_2|)\Delta H \begin{pmatrix} |\Psi_1\rangle \\ |\Psi_2\rangle \end{pmatrix} = vp_y sgn(B)\sigma_z. \tag{2.46}$$

The sign dependence of B in the effective model also reflects the fact that the helical edge states disappear if $B = 0$. The dispersion relations for the bound states at the boundary are

$$\epsilon_{p_y,\pm} = \pm vp_y. \tag{2.47}$$

Electrons have positive $(+v)$ and negative velocity $(-v)$ in their two different states, respectively, and form a pair of helical edge states.

The exact solutions of the edge states in this two-dimensional equation have the form similar to that in the one-dimensional equation [5],

$$\Psi_1 = \frac{C}{\sqrt{2}} \begin{pmatrix} sgn(B) \\ 0 \\ 0 \\ i \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-}) e^{+ip_y y/\hbar} \tag{2.48}$$

and

$$\Psi_2 = \frac{C}{\sqrt{2}} \begin{pmatrix} 0 \\ sgn(B) \\ i \\ 0 \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-}) e^{+ip_y y/\hbar}, \tag{2.49}$$

with the dispersion relations $\epsilon_{p_y,\pm} = \pm v p_y \mathrm{sgn}(B)$. The characteristic lengths become p_y dependent,

$$\xi_\pm^{-1} = \frac{v}{2\,|B|\,\hbar} \left(1 \pm \sqrt{1 - 4mB + 4B^2 p_y^2/v^2}\right). \tag{2.50}$$

In two dimensions, the Chern number or Thouless-Kohmoto-Nightingale-Nijs (TKNN) integer can be used to characterize whether the system is topologically trivial or non-trivial [6]. For the two-band Hamiltonian in the form $H = \mathbf{d}(p) \cdot \sigma$, the Chern number is expressed as

$$n_c = -\frac{1}{4\pi} \int d\mathbf{p} \frac{\mathbf{d} \cdot (\partial_{p_x} \mathbf{d} \times \partial_{p_y} \mathbf{d})}{d^3}, \tag{2.51}$$

where $d^2 = \sum_{\alpha=x,y,z} d_\alpha^2$ (see Appendix A.2). The integral runs over the first Brillouin zone for a lattice system, in which the number n_c is always an integer (see Appendix A.1). In the continuous limit, the integral area becomes infinite, the integral can be fractional. For (2.45), the Chern number has the form [7, 8]

$$n_\pm = \pm \frac{1}{2}(sgn(m) + sgn(B)), \tag{2.52}$$

which is related to the Hall conductance $\sigma_\pm = n_\pm e^2/h$. When m and B have the same sign, $n_\pm = \pm 1$, and the system is topologically non-trivial. But if m and B have different signs, $n_\pm = 0$. The topologically non-trivial condition is in agreement with the existence condition of the edge state solution $mB > 0$. This reflects the bulk-edge relation of the integer quantum Hall effect [9].

2.5.3 Three Dimensions: Surface States

In three dimensions, we consider a y–z plane at $x = 0$. We can derive an effective model for the surface states by means of the one-dimensional solution of the bound state. As the momenta among the y–z plane are good quantum numbers, we use their eigenvalues to replace the momentum operators, p_y and p_z. Consider p_y and p_z dependent part as a perturbation to $H_{1D}(x)$,

$$\Delta H_{3D} = vp_y\alpha_y + vp_z\alpha_z - B(p_y^2 + p_z^2)\beta. \tag{2.53}$$

The solutions of the three-dimensional Dirac equation at $p_y = p_z = 0$ are identical to the two one-dimensional solutions, $|\Psi_1\rangle$ and $|\Psi_2\rangle$ in (2.43) and (2.44). For p_y, $p_z \neq 0$, we use the solutions

$$\Psi_1 = \frac{C}{\sqrt{2}} \begin{pmatrix} sgn(B) \\ 0 \\ 0 \\ i \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-})e^{i(p_y y + p_z z)/\hbar} \tag{2.54}$$

and

$$\Psi_2 = \frac{C}{\sqrt{2}} \begin{pmatrix} 0 \\ sgn(B) \\ i \\ 0 \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-})e^{i(p_y y + p_z z)/\hbar} \tag{2.55}$$

as the basis. A straightforward calculation as in the two-dimensional case gives

$$H_{eff} = (\langle\Psi_1| \,, \langle\Psi_2|)\Delta H_{3D} \begin{pmatrix} |\Psi_1\rangle \\ |\Psi_2\rangle \end{pmatrix} = vsgn(B)(p \times \sigma)_x. \tag{2.56}$$

Under a unitary transformation,

$$\Phi_1 = \frac{1}{\sqrt{2}}(|\Psi_1\rangle - i\,|\Psi_2\rangle) \tag{2.57}$$

and

$$\Phi_2 = \frac{-i}{\sqrt{2}}(|\Psi_1\rangle + i\,|\Psi_2\rangle), \tag{2.58}$$

one can have a gapless Dirac equation for the surface states

$$\begin{aligned} H_{eff} &= \frac{1}{2}(\langle\Phi_1|, \langle\Phi_2|)\Delta H_{3D}\begin{pmatrix}|\Phi_1\rangle \\ |\Phi_2\rangle\end{pmatrix} \\ &= vsgn(B)(p_y\sigma_y + p_z\sigma_z). \end{aligned} \tag{2.59}$$

The dispersion relations become $\epsilon_{p,\pm} = \pm vp$ with $p = \sqrt{p_y^2 + p_z^2}$. In this way, we have an effective model for a single Dirac cone of the surface states as plotted in Fig. 2.4. Note that σ_i in the Hamiltonian is not a real spin, which is determined by two states at $p_y = p_z = 0$. In some systems $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are almost polarized along the z-direction of the electron spin. In this sense, the Pauli matrices in (2.56) may be regarded as approximating a real spin.

The exact solutions of the surface states of this three-dimensional equation with a boundary are

$$\Psi_\pm = C\Psi_\pm^0(e^{-x/\xi_+} - e^{-x/\xi_-})\exp[+i\left(p_y y + p_z z\right)/\hbar], \tag{2.60}$$

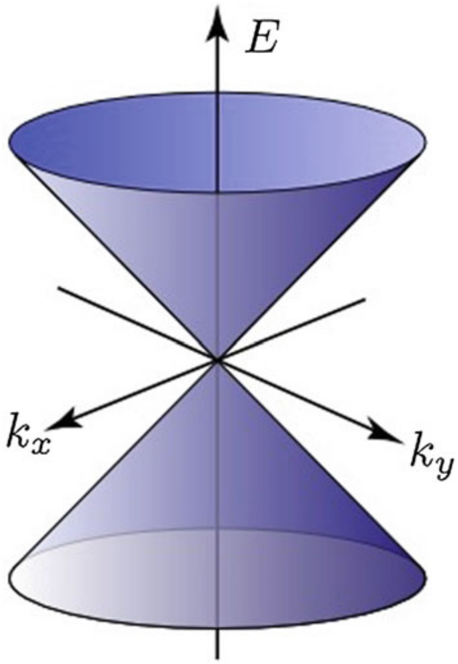

Fig. 2.4 The Dirac cone of the surface states in momentum space

where

$$\Psi_+^0 = \begin{pmatrix} \cos\frac{\theta}{2} sgn(B) \\ -i\sin\frac{\theta}{2} sgn(B) \\ \sin\frac{\theta}{2} \\ i\cos\frac{\theta}{2} \end{pmatrix} \tag{2.61}$$

and

$$\Psi_-^0 = \begin{pmatrix} \sin\frac{\theta}{2} sgn(B) \\ i\cos\frac{\theta}{2} sgn(B) \\ -\cos\frac{\theta}{2} \\ i\sin\frac{\theta}{2} \end{pmatrix} \tag{2.62}$$

with the dispersion relation $\epsilon_{p,\pm} = \pm vp\text{sgn}(B)$. $\tan\theta = p_y/p_z$. The penetration depth becomes p dependent,

$$\xi_\pm^{-1} = \frac{v}{2\,|B|\,\hbar}\left(1 \pm \sqrt{1 - 4mB + 4B^2p^2/\hbar^2}\right). \tag{2.63}$$

2.5.4 Generalization to Higher-Dimensional Topological Insulators

The solution can be generalized to higher-dimensional system. We conclude that there is always a (d-1)-dimensional surface state in the d-dimensional modified Dirac equation when $mB > 0$.

2.6 Summary

From the solutions of the modified Dirac equation, we found the following conclusions under the condition of $mB > 0$,

- in one dimension, there exists a bound state of zero energy near the end;
- in two dimensions, there exists solution of a pair of helical edge states near the edge;
- in three dimensions, there exists solution of surface states near the surface; and
- in higher dimensions, there always exists a higher dimensional boundary states.

From the solutions of the bound states near the boundary and the calculation of the Z_2 index, we conclude that the modified Dirac equation can provide a description of a large class of topological insulators from one to higher dimensions.

2.7 Further Reading

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