

# TOPOLOGICAL INSULATOR AND THE DIRAC EQUATION

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We present a general description of topological insulators from the point of view of Dirac equations. The  $Z_2$  index for the Dirac equation is always zero, and thus the Dirac equation is topologically trivial. After the quadratic term in momentum is introduced to correct the mass term  $m$  or the band gap of the Dirac equation, i.e.,  $m \rightarrow m - Bp^2$ , the  $Z_2$  index is modified as 1 for  $mB > 0$  and 0 for  $mB < 0$ . For a fixed  $B$  there exists a topological quantum phase transition from a topologically trivial system to a non-trivial system when the sign of mass  $m$  changes. A series of solutions near the boundary in the modified Dirac equation are obtained, which is characteristic of topological insulator. From the solutions of the bound states and the  $Z_2$  index we establish a relation between the Dirac equation and topological insulators.

*Keywords:* Spintronics; Topological insulator; Dirac equation.

## 1. Introduction

Translational invariance in crystal lattices and the Bloch theorem for the wavefunction of electrons in solid make it possible for us to know the band structures of solid and why a solid is metal, insulator or semiconductor. Recent years it is found that a new class of materials possesses a feature that its bulk is insulating while its surface or edge is metallic. This metallic behavior is quite robust against impurities or interaction, and is protected by the intrinsic symmetry of the band structures of electrons. The materials with this new feature are called topological insulator.<sup>1-3</sup>

In 1979 the one-parameter scaling theory predicted that all electrons in systems of two or lower dimension should be localized for a weak disorder.<sup>4</sup> This theory shaped the research of lower dimensional systems with disorders or interaction. Almost at the same time, von Klitzing *et al* discovered experimentally integer quantum Hall effect (IQHE)

in two-dimensional (2D) electron gas in semiconductor heterojunction in a strong magnetic field, in which longitudinal conductance becomes zero while the quantum plateau of the Hall conductance appears at  $\nu e^2/h$  ( $\nu$  is an integer).<sup>5</sup> Two years later Tsui *et al* observed the fractional quantum Hall effect (FQHE) in a sample with higher mobility.<sup>6</sup> In the theory of edge states for IQHE electrons form discrete Landau levels in a strong magnetic field. Electrons in the bulk have a vanishing group velocity, and are easily localized by impurities or disorder while the electrons near the boundary are skipping along the boundary to form a conducting channel.<sup>7, 8</sup> Thus in IQHE all bulk electrons are localized to be insulating while the edge electrons form several conducting channels according to the electron density which is robust against the impurities. This feature indicates that IQHE is a new state of quantum matter, i.e., one of topological insulators. In FQHE it is the electron-electron interaction that makes electrons incompressible and form

stable metallic edge states.<sup>9, 10</sup> The quasiparticles in FQHE have fractional charges, and obey new quantum statistics. In 1988 Haldane proposed that IQHE could be realized in a lattice system of spinless fermions in a periodic magnetic flux.<sup>11</sup> Though the total magnetic flux is zero, electrons are driven to form an conducting edge channel by the local magnetic flux. Since there is no pure magnetic field the quantum Hall conductance originates from the band structure of fermions in the lattice instead of the discrete Landau levels.

In 2005 Kane and Mele generalized the Haldane's model to a lattice of spin 1/2 electrons.<sup>12</sup> The strong spin-orbit coupling, an effect of relativistic quantum mechanics for electrons in atoms, is introduced to replace the periodic magnetic flux in Haldane's model. This interaction looks like a spin-dependent magnetic field to act on electron spins. Different electron spins experience opposite spin-orbit force, i.e., spin transverse force.<sup>13</sup> As a result, a bilayer Haldane model may be realized in a spin- $\frac{1}{2}$  electron system with spin-orbit coupling, which exhibits quantum spin Hall effect (QSHE). In the case there exist spin-dependent edge states around the boundary of the system, i.e., electrons with different spins move in opposite directions, and form a pair of helical edge states. In this system the time-reversal symmetry is preserved, and the edge states are robust against impurities or disorders because the electron backscattering in the two edge channels is prohibited due to the symmetry. Bernevig, Hughes and Zhang predicted that the QSHE effect can be realized in the HgTe/CdTe quantum well.<sup>14</sup> HgTe is an inverted-band material, and CdTe is a normal band one. Tuning the thickness of HgTe layer may lead to the band inversion in the quantum well, which exhibits a topological phase transition.<sup>15, 16</sup> This prediction was confirmed experimentally by König *et al* soon after the prediction.<sup>17</sup> The stability of the QSHE was studied by several groups.<sup>18–21</sup> Li *et al* discovered that the disorder may even generate QSHE, and proposed a possible realization of topological Anderson insulator, in which all bulk electrons are localized by impurities meanwhile a conducting helical edge channels appears.<sup>22</sup> This phase was studied numerically and analytically.<sup>23, 24</sup> Strong Coulomb interactions may also generate QSHE in Mott insulators.<sup>25, 26</sup>

The generalization of QSHE to three dimension is topologically non-trivial.<sup>27–30</sup> Kane and Mele proposed a  $Z_2$  index to classify the materials with

time-reversal invariance into a strong or weak topological insulator.<sup>31</sup> For a strong topological insulator, there exists an odd number of surface states crossing the Fermi surface of the system. The backscattering of electrons in the surface states is prohibited because of the time-reversal symmetry.  $\text{Bi}_{1-x}\text{Sb}_x$  was predicted to be 3D topological insulator by Fu and Kane<sup>32</sup> and was verified experimentally.<sup>33</sup> Zhang *et al*<sup>34</sup> and Xia *et al*<sup>35</sup> pointed out that  $\text{Bi}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$  are topological insulators with a single Dirac cone of the surface states. ARPES data showed clearly the existence of single Dirac cone in  $\text{Bi}_2\text{Se}_3$ <sup>35</sup> and  $\text{Bi}_2\text{Te}_3$ .<sup>36</sup> Electrons in the surface states possess a quantum spin texture structure, and electron momenta are coupled strongly with electron spins. These result in a lot of exotic magnetoelectric properties. Qi *et al.*<sup>37</sup> proposed the unconventional magnetoelectric effect for the surface states, in which electric and magnetic fields are coupled together and are governed by so-call "axion equation" instead of Maxwell equations. It is regarded as one of the characteristic features of the topological insulators.<sup>38, 39</sup> Fu and Kane proposed a possible realization of Majorana fermions as a proximity effect of *s*-wave superconductor and surface states of topological insulator.<sup>40</sup> The Majorana fermions are topologically protected from local sources of decoherence, and will be of potential application in universal quantum computation.<sup>41, 42</sup> Thus the topological insulators open a new route to explore novel and exotic quantum particles in condensed matters.

The Dirac equation is a relativistic quantum mechanical equation for elementary spin- $\frac{1}{2}$  particle.<sup>43, 44</sup> It enters the field of topological insulator in two aspects. Firstly, the band structures of topological insulators are topologically non-trivial because of strong spin-orbit coupling, while the Dirac equation provides a description that couples spin, momentum and external fields together.<sup>45</sup> Secondly, the Dirac equation has the same mathematical structure of the effective Hamiltonian to the QSHE and 3D topological insulators, which are derived from the expansion of invariants or the  $\mathbf{k} \cdot \mathbf{p}$  perturbation theory. The difference is that the effective models for topological insulators describe the coupling between electrons in the conduction and valence bands, not the electron and positrons in Dirac's theory.

In this paper we start with the Dirac equation to provide a simple but unified description

for a large family of topological insulators. A series of solvable differential equations are presented to demonstrate the existence of edge and surface states in topological insulators.

## 2. Dirac Equation and Solutions of the Bound States

In 1928, Paul A. M. Dirac wrote down an equation for relativistic quantum mechanical wavefunctions, which describes elementary spin- $\frac{1}{2}$  particles,<sup>43, 44</sup>

$$H = c\mathbf{p} \cdot \boldsymbol{\alpha} + mc^2\beta, \quad (1)$$

where  $m$  is the rest mass of particle and  $c$  is the speed of light.  $\alpha_i$  and  $\beta$  are the Dirac matrices satisfying

$$\alpha_i^2 = \beta^2 = 1, \quad (2a)$$

$$\alpha_i\alpha_j = -\alpha_j\alpha_i, \quad (2b)$$

$$\alpha_i\beta = -\beta\alpha_i. \quad (2c)$$

In two dimensions, the Dirac matrices have the same forms of the Pauli matrices  $\sigma_i$ , i.e.,  $\alpha_x = \sigma_x$ ,  $\alpha_y = \sigma_y$ , and  $\beta = \sigma_z$ . In three dimensions, one representation of the Dirac matrices in terms of the Pauli matrices  $\sigma_i$  ( $i = x, y, z$ ) is

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad (3a)$$

$$\beta = \begin{pmatrix} \sigma_0 & 0 \\ 0 & -\sigma_0 \end{pmatrix}, \quad (3b)$$

where  $\sigma_0$  is a  $2 \times 2$  identity matrix. From this equation, Einstein's relativistic energy-momentum relation will be automatically the solution of the equation,  $E^2 = m^2c^4 + p^2c^2$ . This equation demands the existence of antiparticle, i.e., particle with negative energy or mass, and predicts the existence of positron, the antiparticle of the electron. It is one of the main achievements of modern theoretical physics.

Under the transformation of  $m \rightarrow -m$  it is found that the equation remains invariant if  $\beta \rightarrow -\beta$ , which satisfies all mutual anticommutation relations for  $\alpha_i$  and  $\beta$ . This reflects the symmetry between the positive and negative energy particles.

Possible relation between the Dirac equation and the topological insulator can be seen from a solution of the bound state at the interface between two regions of positive and negative masses. For simplicity, we first consider a one-dimensional (1D) example

$$h(x) = -iv\hbar\partial_x\sigma_x + m(x)v^2\sigma_z, \quad (4)$$

and

$$m(x) = \begin{cases} -m_1, & x < 0; \\ +m_2, & x \geq 0. \end{cases} \quad (5)$$

(and  $m_1$  and  $m_2 > 0$ ). Except for the extended solutions in the whole space, there exists a solution of the bound state with zero energy

$$\Psi(x) = \sqrt{\frac{v}{\hbar} \frac{m_1 m_2}{m_1 + m_2}} \begin{pmatrix} i \\ 1 \end{pmatrix} e^{-|m(x)vx|/\hbar}. \quad (6)$$

The solution dominantly distributes near the point of  $x = 0$  and decays exponentially away from the point of  $x = 0$ . The solution of  $m_1 = m_2$  was first obtained by Jackiw and Rebbi, and is a basis for the fractional charge in one-dimensional system.<sup>46</sup> The solution exists even when  $m_2 \rightarrow +\infty$ . In this case,  $\Psi(x) \rightarrow 0$  for  $x > 0$ . However, we have to point out that the wavefunction does not vanish at the interface when  $m_2 \rightarrow +\infty$ . If we regard the vacuum as a system with an infinite positive mass, a system of a negative mass with an open boundary condition forms a bound state near the boundary. This is the source of some popular pictures for topological insulator.

In 2D, we consider a system with an interface parallel to the  $y$ -axis, with  $m(x) = m_1$  for  $x > 0$ , and  $-m_2$  for  $x < 0$ .  $k_y$  is a good quantum number. We have two solutions whose wavefunctions dominantly distribute around the interface. One solution has the form

$$\Psi(x, k_y) = \sqrt{\frac{v}{\hbar} \frac{m_1 m_2}{m_1 + m_2}} \begin{pmatrix} i \\ 0 \\ 0 \\ 1 \end{pmatrix} e^{-|m(x)vx|/\hbar + ik_y y}, \quad (7)$$

with the dispersion  $\epsilon_k = v\hbar k_y$ . The other one has the form

$$\Psi(x, k_y) = \sqrt{\frac{v}{\hbar} \frac{m_1 m_2}{m_1 + m_2}} \begin{pmatrix} 0 \\ i \\ 1 \\ 0 \end{pmatrix} e^{-|m(x)vx|/\hbar + ik_y y}, \quad (8)$$

with the dispersion  $\epsilon_k = -v\hbar k_y$ . Both states carry a current along the interface, but electrons move in opposite directions. The currents decay exponentially away from the interface. As the system does not break the time-reversal symmetry, the two states are counterpart with time-reversal symmetry with each other. This is a pair of helical edge (or bound) states at the interface.

In 3D, we can also find a solution for the surface states. The dispersion relation for the surface

states is  $\epsilon_p = \pm vp$ . It has a rotational symmetry and forms a Dirac cone.

From these solutions we found that the edge states and surface states exist at the interface of systems with positive and negative masses. However, since there is a positive-negative mass symmetry in the Dirac equation, we cannot simply say which one is topologically trivial or non-trivial. Thus the Dirac equation alone is not enough to describe the topological insulators.

### 3. Modified Dirac equation and $Z_2$ topological invariant

To explore the topological insulator, we start with a modified Dirac Hamiltonian by introducing a quadratic correction  $-Bp^2$  in momentum  $\mathbf{p}$  to the band gap or rest energy term,

$$H = v\mathbf{p} \cdot \alpha + (mv^2 - B\mathbf{p}^2)\beta, \quad (9)$$

where  $mv^2$  is the band gap of particle and  $m$  and  $v$  have dimensions of mass and speed, respectively. The quadratic term breaks the mass symmetry in the Dirac equation, and makes this equation topologically distinct from the original one.

The general solutions of the wavefunctions can be expressed as  $\Psi_\nu = u_\nu(p)e^{i(\mathbf{p}\cdot\mathbf{r} - E_{p,\nu}t)/\hbar}$ . The dispersion relations of four energy bands are  $E_{p,\nu(=1,2)} = -E_{p,\nu(=3,4)} = \sqrt{v^2p^2 + (mv^2 - Bp^2)^2}$ . The four-component spinors  $u_\nu(p)$  can be expressed as  $u_\nu(p) = Su_\nu(p=0)$  with

$$S = \sqrt{\frac{\epsilon_p}{2E_{p,1}}} \begin{pmatrix} 1 & 0 & -\frac{p_z v}{\epsilon_p} & -\frac{p_- v}{\epsilon_p} \\ 0 & 1 & -\frac{p_+ v}{\epsilon_p} & \frac{p_z v}{\epsilon_p} \\ \frac{p_z v}{\epsilon_p} & \frac{p_- v}{\epsilon_p} & 1 & 0 \\ \frac{p_+ v}{\epsilon_p} & -\frac{p_z v}{\epsilon_p} & 0 & 1 \end{pmatrix}, \quad (10)$$

where  $p_\pm = p_x \pm ip_y$ ,  $\epsilon_p = E_{p,1} + (mv^2 - Bp^2)$ , and  $u_\nu(0)$  is one of the four eigenstates of the  $\beta$  matrix.

The topological properties of the modified Dirac equation can be obtained from these free-particle solutions. The Dirac equation is invariant under the time-reversal symmetry, and can be classified according to the  $Z_2$  topological classification.<sup>31</sup> In the representation that the Dirac matrices can be written as Eq. (3), the time-reversal operator is defined as<sup>47</sup>  $\Theta \equiv -i\alpha_x \alpha_z \mathcal{K}$ , where  $\mathcal{K}$  is the complex conjugation operator. Under the time-reversal operation, the modified Dirac equation remains invariant, i.e.,  $\Theta H(p)\Theta^{-1} = H(-p)$  ( $p$  is the momentum quantum number). Furthermore we have relations that  $\Theta u_1(p) = -iu_2(-p)$  and

$\Theta u_2(p) = +iu_1(-p)$ , where  $\Theta$  satisfies that  $\Theta^2 = -1$ . Similarly,  $\Theta u_3(p) = -iu_4(-p)$  and  $\Theta u_4(p) = +iu_3(-p)$ . Thus the solutions of  $\{u_1(p), u_2(-p)\}$  and  $\{u_3(p), u_4(-p)\}$  are two degenerate Kramer pairs of positive and negative energies, respectively. The matrix of overlap  $\{\langle u_\mu(p) | \Theta | u_\nu(p) \rangle\}$  has the form

$$\begin{pmatrix} 0 & i\frac{mv^2 - Bp^2}{E_{p,1}} & -i\frac{p_- v}{E_{p,1}} & i\frac{p_z v}{E_{p,1}} \\ -i\frac{mv^2 - Bp^2}{E_{p,1}} & 0 & i\frac{p_z v}{E_{p,1}} & i\frac{p_+ v}{E_{p,1}} \\ i\frac{p_- v}{E_{p,1}} & -i\frac{p_z v}{E_{p,1}} & 0 & i\frac{mv^2 - Bp^2}{E_{p,1}} \\ -i\frac{p_z v}{E_{p,1}} & -i\frac{p_+ v}{E_{p,1}} & -i\frac{mv^2 - Bp^2}{E_{p,1}} & 0 \end{pmatrix}, \quad (11)$$

which is antisymmetric, i.e.,  $\langle u_\mu(p) | \Theta | u_\nu(p) \rangle = -\langle u_\nu(p) | \Theta | u_\mu(p) \rangle$ . For the two negative energy bands  $u_3(p)$  and  $u_4(p)$ , the submatrix of overlap can be expressed by  $\epsilon_{\mu\nu}P(\mathbf{p})$ , in terms of the Pfaffian

$$P(\mathbf{p}) = i\frac{mv^2 - Bp^2}{\sqrt{(mv^2 - Bp^2)^2 + v^2p^2}}. \quad (12)$$

According to Kane and Mele,<sup>31</sup> the even or odd number of pairs of the zeros in  $P(\mathbf{p})$  defines the  $Z_2$  topological invariant. Here we want to emphasize that the sign of a dimensionless parameter  $mB$  will determine the  $Z_2$  invariant of the modified Dirac equation. Since  $P(\mathbf{p})$  is always non-zero for  $mB \leq 0$  and there exists no zero in the Pfaffian, we conclude immediately that the modified Dirac Hamiltonian for  $mB \leq 0$  as well as the conventional Dirac Hamiltonian ( $B = 0$ ) are topologically trivial.

For  $mB > 0$  the case is different. In this continuous model, the Brillouin zone becomes infinite. At  $p = 0$  and  $p = +\infty$ ,  $P(0) = i\text{sgn}(m)$  and  $P(+\infty) = -i\text{sgn}(B)$ . In this case  $P(\mathbf{p}) = 0$  at  $p^2 = mv^2/B$ .  $\mathbf{p} = 0$  is always one of the time-reversal invariant momenta (TRIM). As a result of an isotropic model in the momentum space, we can think all points of  $p = +\infty$  shrink into one point if we regard the continuous model as a limit of the lattice model by taking the lattice space  $a \rightarrow 0$  and the reciprocal lattice vector  $G = 2\pi/a \rightarrow +\infty$ . In this sense as a limit of a square lattice other three TRIMs have  $P(0, G/2) = P(G/2, 0) = P(G/2, G/2) = P(+\infty)$  which has an opposite sign of  $P(0)$  if  $mB > 0$ . Similarly for a cubic lattice  $P(\mathbf{p})$  of other seven TRIMs have opposite signs of  $P(0)$ . Following Fu, Kane and Mele,<sup>27, 32</sup> we conclude that:

*The modified Dirac Hamiltonian is topologically non-trivial only if  $mB > 0$ .*

In two dimensions  $Z_2$  index can be determined by evaluating the winding number of the phase of

$P(\mathbf{p})$  around a loop of enclosing half the Brillouin zone in the complex plane of  $\mathbf{p} = p_x + ip_y$ ,

$$I = \frac{1}{2\pi i} \oint_{\mathcal{C}} d\mathbf{p} \cdot \nabla_{\mathbf{p}} \log[P(\mathbf{p}) + i\delta]. \quad (13)$$

Because the model is isotropic, the integral then reduces to the path only along  $p_x$ -axis while the part of the half-circle integral vanishes for  $\delta > 0$  and  $|\mathbf{p}| \rightarrow +\infty$ . Along the  $p_x$  axis only one of a pair of zeros in the ring is enclosed in the contour  $\mathcal{C}$  when  $mB > 0$ , which gives a  $Z_2$  index  $I = 1$ . This defines the non-trivial QSH phase.

#### 4. Topological invariants and quantum phase transition

An alternative approach to explore the topological property of the Dirac model is the Green function method.<sup>48</sup> Volovik<sup>49</sup> proposed that the Green function rather than the Hamiltonian is more applicable to classify topological insulators.

For one block of a two-dimensional Dirac equation,  $H = v\mathbf{p} \cdot \boldsymbol{\sigma} + (mv^2 - Bp^2)\sigma_z$ , the time-reversal symmetry is broken. The Green function has the form

$$\begin{aligned} G(i\omega_n, p) &= \frac{1}{i\omega_n - H} \\ &= -\frac{v\mathbf{p} \cdot \boldsymbol{\sigma} + (mv^2 - Bp^2)\sigma_z + i\omega_n}{\omega_n^2 + h^2(p)}, \end{aligned}$$

where  $h^2(k) = H^2 = v^2p^2 + (mv^2 - Bp^2)^2$ . The topological invariant is defined as

$$n = \frac{\epsilon_{ijk}}{24\pi^2} \text{Tr} \left[ \int d\mathbf{p} dp_0 G \partial_{p_i} G^{-1} G \partial_{p_j} G^{-1} G \partial_{p_k} G^{-1} \right], \quad (14)$$

where  $i, j, k = 0, 1, 2$  and  $p_0 = i\omega_n$ . After carrying out the frequency integral explicitly, one obtains the TKNN invariant in terms of the Berry curvature<sup>51</sup>

$$n = \frac{1}{2\pi} \int d\mathbf{p} [\nabla_{\mathbf{p}} \times \mathbf{A}(\mathbf{p})], \quad (15)$$

where

$$\mathbf{A}(\mathbf{p}) = i \langle u_c(\mathbf{p}) | \nabla_{\mathbf{p}} | u_c(\mathbf{p}) \rangle, \quad (16)$$

and  $|u_c(\mathbf{p})\rangle$  is the occupied state. The TKNN invariant is the Chern number

$$n = -\frac{1}{2} [\text{sgn}(m) + \text{sgn}(B)].$$

From this formula, we have two topological non-trivial phases with  $n = \pm 1$  for  $mB > 0$ , and topologically trivial phase with  $n = 0$ . We also have

two marginal phases with  $n = \pm 1/2$  for  $m = 0$  or  $B = 0$ . The free Dirac fermions of  $B = 0$  are marginal phases. At the junction of two systems with opposite signs of mass  $m$ , the topological invariant changes by  $\delta n = 1$  or  $-1$ . Thus there exists a boundary state at the junction. For the gapless Dirac fermions  $m = 0$  and  $B \neq 0$ , the system is also marginal. The topological invariant also changes by  $\delta n = 1$  at the interface between positive and negative  $B$ .

In 3D we have to consider  $4 \times 4$  Dirac Hamiltonian, the Green function has the form

$$\begin{aligned} G(i\omega_n, p) &= \frac{1}{i\omega_n - H} \\ &= -\frac{v\mathbf{p} \cdot \boldsymbol{\alpha} + (mv^2 - Bp^2)\beta + i\omega_n}{\omega_n^2 + h^2(p)}. \end{aligned}$$

There is the following symmetry-protected topological invariant

$$\begin{aligned} \tilde{N} &= \\ &= \frac{\epsilon_{ijk}}{24\pi^2} \text{Tr} [K_{i\omega_n=0} \int d\mathbf{p} G \partial_{p_i} G^{-1} G \partial_{p_j} G^{-1} G \partial_{p_k} G^{-1}], \end{aligned} \quad (17)$$

where  $K = \sigma_y \otimes \sigma_0$  is the symmetry-related operator. After tedious algebra, it is found that

$$\tilde{N} = \text{sgn}(m) + \text{sgn}(B). \quad (18)$$

When  $mB > 0$ ,  $\tilde{N} = \pm 2$ , which defines the phase topologically non-trivial. If  $B$  is fixed to be positive, there exists a quantum phase transition from topologically trivial phase of  $m < 0$  to a topologically non-trivial phase of  $m > 0$ . This is in good agreement with the result of  $Z_2$  index in the preceding section.

Except for the phases of  $\tilde{N} = \pm 2$ , it is found that there exists a marginal topological phase of  $\tilde{N} = \pm 1$ . For free Dirac fermions of  $B = 0$ , the topological invariant  $\tilde{N} = \text{sgn}(m)$ . It is  $+1$  for a positive mass and  $-1$  for a negative mass. Their difference is  $\Delta\tilde{N} = 2$ , which is the origin of the existence of the bound states at the interface of two systems with positive and negative mass as we discussed in Section 2. There exist intermediate gapless phases of  $m = 0$  between topological nontrivial ( $\tilde{N} = \pm 2$ ) and trivial ( $\tilde{N} = 0$ ) phases. At the critical point of topological quantum phase transition, all intermediate states are gapless. Its topological invariant is also  $\tilde{N} = +1$  or  $-1$  just like the free Dirac fermions.

## 5. The topologically protected boundary states

### 5.1. 1D: the bound state of zero energy

Let us start with the 1D case. In this case, the Hamiltonian in Eq. (9) can be decoupled into two sets of independent blocks in the form

$$h(x) = vp_x\sigma_x + (mv^2 - Bp_x^2)\sigma_z. \quad (19)$$

For a semi-infinite chain, we consider an open boundary condition at  $x = 0$ . We may have a series of extended solutions which spread in the whole space. In this section we focus on the solutions of bound states near the end of the chain. We require that the wavefunction vanishes at  $x = +\infty$ . In the condition of  $mB > 0$ , there exists a solution of the bound state with zero energy

$$\begin{aligned} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} &= \frac{C}{\sqrt{2}} \begin{pmatrix} \text{sgn}(B) \\ i \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-}), \\ \xi_{\pm}^{-1} &= \frac{v}{2|B|\hbar} \left(1 \pm \sqrt{1 - 4mB}\right), \end{aligned} \quad (20)$$

where  $C$  is the normalization constant. The main feature of this solution is that the wavefunction dominantly distributes near the boundary. The two parameters  $\xi_- > \xi_+$  are very important length scales, they decide the spatial distribution of the wavefunction and characterize the bound state. When  $B \rightarrow 0$ ,  $\xi_+ \rightarrow |B|\hbar/v$  and  $\xi_- = \hbar/mv$ , i.e.,  $\xi_+$  approaches to zero, and  $\xi_-$  becomes a finite constant. If we relax the constraint of the vanishing wavefunction 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 arrive at the same conclusion.

In the four-component form of Eq. (9), two degenerate solutions have the form,

$$\Psi_1 = \frac{C}{\sqrt{2}} \begin{pmatrix} \text{sgn}(B) \\ 0 \\ 0 \\ i \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-}), \quad (21a)$$

$$\Psi_2 = \frac{C}{\sqrt{2}} \begin{pmatrix} 0 \\ \text{sgn}(B) \\ i \\ 0 \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-}). \quad (21b)$$

### 5.2. 2D: the helical edge states

In two dimensions, the Hamiltonian is decoupled into two independent blocks

$$h_{\pm} = vp_x\sigma_x \pm vp_y\sigma_y + (mv^2 - Bp^2)\sigma_z. \quad (22)$$

These two subsets break the ‘‘time’’ reversal symmetry under the transformation of  $\sigma_i \rightarrow -\sigma_i$  and  $p_i \rightarrow -p_i$ .

We consider a semi-infinite plane with the boundary at  $x = 0$ .  $p_y$  is a good quantum number. At  $p_y = 0$ , the 2D equation has the same form as the 1D equation. The  $x$ -dependent part of the solutions of bound states has the identical form as in 1D. Thus we use the two 1D solutions  $\{\Psi_1, \Psi_2\}$  as the basis. The  $y$ -dependent part  $\Delta H_{2D} = vp_y\alpha_y - Bp_y^2\beta$  is regarded as the perturbation to the 1D Hamiltonian. In this way, we have a 1D effective model for the helical edge states

$$H_{\text{eff}} = (\langle\Psi_1|, \langle\Psi_2|)\Delta H \begin{pmatrix} |\Psi_1\rangle \\ |\Psi_2\rangle \end{pmatrix} = vp_y\text{sgn}(B)\sigma_z. \quad (23)$$

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

$$\epsilon_p = \pm vp_y. \quad (24)$$

Electrons will have positive ( $+v$ ) and negative velocity ( $-v$ ) in two different states, respectively, and form a pair of helical edge states. Thus the 2D equation can describe the quantum spin Hall system.

The exact solutions of the edge states to this 2D equation have the similar form of 1D<sup>50</sup>

$$\Psi_1 = \frac{C}{\sqrt{2}} \begin{pmatrix} \text{sgn}(B) \\ 0 \\ 0 \\ i \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-})e^{+ip_y y/\hbar}, \quad (25a)$$

$$\Psi_2 = \frac{C}{\sqrt{2}} \begin{pmatrix} 0 \\ \text{sgn}(B) \\ i \\ 0 \end{pmatrix} (e^{-x/\xi_+} - e^{-x/\xi_-})e^{+ip_y y/\hbar}, \quad (25b)$$

with the dispersion relation  $E_{p_y} = \pm vp_y\text{sgn}(B)\sigma_z$ . The penetration depth becomes  $p_y$  dependent,

$$\xi_{\pm}^{-1} = \frac{v}{2|B|\hbar} \left(1 \pm \sqrt{1 - 4mB + 4B^2p_y^2/v^2}\right). \quad (26)$$

In two-dimension, the Chern number or Thouless-Kohmoto-Nightingale-Nijs integer can be used to characterize whether the system is topologically trivial or non-trivial.<sup>51</sup> Writing the Hamiltonian Eq. (22) in the form  $H = \mathbf{d}(p) \cdot \sigma$ , the Chern number is expressed as

$$n_c = \int \frac{d\mathbf{p}}{(2\pi\hbar)^2} \frac{\epsilon_{ijk} d_i \frac{\partial d_j}{\partial p_x} \frac{\partial d_k}{\partial p_y}}{d^3}, \quad (27)$$

where  $d^2 = \sum_{\alpha=x,y,z} d_\alpha^2$ .<sup>51, 52</sup> The integral runs over the first Brillouin zone for a lattice system. The number is always an integer for a finite first Brillouin zone, but can be fractional for an infinite zone. For these two equations the Chern number has the form<sup>54, 53</sup>

$$n_\pm = \pm[\text{sgn}(m) + \text{sgn}(B)]/2, \quad (28)$$

which gives the Hall conductance  $\sigma_\pm = n_\pm e^2/h$ . When  $m$  and  $B$  have the same sign,  $n_\pm$  becomes  $\pm 1$ , and the systems are 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 edge state solution. This reflects the bulk-edge correspondence of integer quantum Hall effect.<sup>55</sup>

### 5.3. 3D: the surface states

In 3D, we consider a  $y$ - $z$  plane at  $x = 0$ . We can derive an effective model for the surface states by means of the 1D solutions of the bound states. Consider  $p_y$ - and  $p_z$ -dependent part as a perturbation to 1D  $H_{1D}(x)$ ,

$$\Delta H_{3D} = vp_y \alpha_y + vp_z \alpha_z - B(p_y^2 + p_z^2)\beta. \quad (29)$$

The solutions of 3D Dirac equation at  $p_y = p_z = 0$  are identical to the two 1D solutions. A straightforward calculation as in the 2D case gives

$$H_{\text{eff}} = (\langle \Psi_1 |, \langle \Psi_2 |) \Delta H_{3D} \begin{pmatrix} |\Psi_1\rangle \\ |\Psi_2\rangle \end{pmatrix} = v \text{sgn}(B) (p \times \sigma)_x. \quad (30)$$

Under a unitary transformation,

$$\Phi_1 = \frac{1}{\sqrt{2}} (|\Psi_1\rangle - i|\Psi_2\rangle), \quad (31a)$$

$$\Phi_2 = \frac{-i}{\sqrt{2}} (|\Psi_1\rangle + i|\Psi_2\rangle), \quad (31b)$$

we can have a gapless Dirac equation for the surface states

$$H_{\text{eff}} = \frac{1}{2} (\langle \Phi_1 |, \langle \Phi_2 |) \Delta H_{3D} \begin{pmatrix} |\Phi_1\rangle \\ |\Phi_2\rangle \end{pmatrix} = v \text{sgn}(B) (p_y \sigma_y + p_z \sigma_z). \quad (32)$$

The dispersion relations become  $E_p = \pm vp$ . In this way we have an effective model for a single Dirac cone of the surface states.

The exact solutions of the surface states to this 3D equation with the boundary are

$$\Psi_\pm = C \Psi_\pm^0 (e^{-x/\xi_+} - e^{-x/\xi_-}) \exp[+i(p_y y + p_z z)/\hbar], \quad (33a)$$

where

$$\Psi_+^0 = \begin{pmatrix} \cos \frac{\theta}{2} \text{sgn}(B) \\ -i \sin \frac{\theta}{2} \text{sgn}(B) \\ \sin \frac{\theta}{2} \\ i \cos \frac{\theta}{2} \end{pmatrix}, \quad (33b)$$

$$\Psi_-^0 = \begin{pmatrix} \sin \frac{\theta}{2} \text{sgn}(B) \\ i \cos \frac{\theta}{2} \text{sgn}(B) \\ -\cos \frac{\theta}{2} \\ i \sin \frac{\theta}{2} \end{pmatrix}, \quad (33c)$$

with the dispersion relation  $E_\pm = \pm v p \text{sgn}(B)$  and  $p = \sqrt{p_y^2 + p_z^2}$ . The penetration depth becomes  $p$  dependent

$$\xi_\pm^{-1} = \frac{v}{2|B|\hbar} \left( 1 \pm \sqrt{1 - 4mB + 4B^2 p^2 / \hbar^2} \right). \quad (34)$$

### 5.4. Generalization to higher dimensional topological insulators

The solution can be generalized to higher dimensions. We conclude that there always exist  $d$ -dimensional boundary states for the  $(d+1)$ -dimensional modified Dirac equation.

## 6. Application to real systems

Now we address the relevance of the modified Dirac model to real materials. Of course we cannot simply apply the Dirac equation to semiconductors explicitly. Usually the band structures of most semiconductors have no particle-hole symmetry. Thus a quadratic term should be introduced into the modified Dirac model. On the other hand the band structure may not be isotropic and the effective velocities along different axes are different. A more general model has the form,

$$H = \epsilon(p_i) + \sum_i v_i p_i \alpha_i + (mv^2 - \sum_i B_i p_i^2) \beta. \quad (35)$$

To have a solution for topological insulator, the additional terms must keep the band gap open. Otherwise it cannot describe an insulator.

The equation in solids can be derived from the theory of invariant or the  $\mathbf{k} \cdot \mathbf{p}$  perturbation theory as an expansion of the momentum  $\mathbf{p}$  near the  $\Gamma$  point. Since under the time-reversal operation,  $\beta \rightarrow \beta$  and  $\alpha \rightarrow -\alpha$ , if we expand a time-reversal invariant Hamiltonian near the  $\Gamma$  point, the zero-order terms should be constant, i.e.,  $\epsilon(0)$  and  $mv^2\beta$ . The first order terms in momentum must be  $\sum_i v_i p_i \alpha_i$  since  $p_i \rightarrow -p_i$  under time-reversal operation. The second order term is  $\sum_i B_i p_i^2 \beta$  and  $\frac{p^2}{2m}$  in  $\epsilon(p_i)$ . The third order term is the cubic term in  $\alpha$ . The summation up to the second order terms gives the modified Dirac equation.

### 6.1. *Complex p-wave spinless superconductor*

A complex  $p$ -wave spinless superconductor has two topologically distinct phases, one is the strong pairing phase and the other is the weak pairing phase.<sup>56, 48</sup> The weak pairing phase is identical to the Moore-Read quantum Hall state.<sup>56</sup> The system can be described by the modified Dirac model. In the BCS mean field theory, the effective Hamiltonian for quasiparticles in this system has the form

$$K_{\text{eff}} = \sum_k \left[ \xi_k c_k^\dagger c_k + \frac{1}{2} (\Delta_k^* c_{-k} c_k + \Delta_k c_k^\dagger c_{-k}^\dagger) \right]. \quad (36)$$

The normalized ground state has the form

$$|\Omega\rangle = \prod_k (u_k + v_k c_k^\dagger c_{-k}^\dagger) |0\rangle, \quad (37)$$

where  $|0\rangle$  is the vacuum state. The Bogoliubov-de Gennes equation for  $u_k$  and  $v_k$  becomes

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \begin{pmatrix} \xi_k & -\Delta_k^* \\ -\Delta_k & -\xi_k \end{pmatrix} \begin{pmatrix} u_k \\ v_k \end{pmatrix}. \quad (38)$$

For complex  $p$ -wave pairing, we take  $\Delta_k$  to be an eigen function of rotations in  $k$  with eigenvalue of two-dimensional angular momentum  $l = 1$ , and thus at small  $k$  it generically takes the form

$$\Delta_k = \Delta(k_x - ik_y); \quad \xi_k = \frac{k^2}{2m} - \mu. \quad (39)$$

In this way the Bogoliubov-de Gennes equation has the exact form of 2D modified Dirac equation

$$H_{\text{eff}} = -\Delta(k_x \sigma_x + k_y \sigma_y) + \left( \frac{k^2}{2m} - \mu \right) \sigma_z. \quad (40)$$

The Chern number of the effective Hamiltonian becomes

$$n = [\text{sgn}(\mu) + \text{sgn}(1/m)] / 2. \quad (41)$$

Since we assume the mass of the spinless particles  $m$  positive, we conclude that for a positive  $\mu (> 0)$  the Chern number is  $+1$  and for a negative  $\mu$  the Chern number is  $0$ . For  $\mu = 0$ , the Chern number is equal to one half, which is similar to the case of  $m \rightarrow +\infty$  and a finite  $\mu$ . If the quadratic term in  $\xi_k$  is neglected, we see that the topological property will change completely.

Usually for a positive  $\mu$ , the system is in a weak pairing phase, for a negative  $\mu$  the strong coupling phase. Including the quadratic term in  $\xi_k$  we conclude that the weak pairing phase for positive  $\mu$  is a typical topological insulator, which possesses a chiral edge state if the system has a boundary. The exact solution of this equation can be found in the paper by Zhou *et al.*<sup>50</sup> Read and Green<sup>56</sup> argued that a bound state solution exists at a straight domain wall parallel to the  $y$ -axis, with  $\mu(r) = \mu(x)$  small and positive for  $x > 0$ , and negative for  $x < 0$ . There is only one solution for each  $k_y$  so we have a chiral Majorana fermions on the domain wall. From the 2D solution, the system in a weak pairing phase should have a topologically protected and chiral edge state of Majorana fermion. Recently Fu and Kane proposed that due to the superconducting proximity effect the interface of the surface state of three-dimensional topological insulator and an  $s$ -wave superconductor resembles a spinless  $p_x + ip_y$  superconductor, but does not break time-reversal symmetry.<sup>40</sup> The state supports Majorana bound states at vortices.

### 6.2. *Quantum Spin Hall Effect: HgTe/CdTe quantum well and thin film of topological insulator*

In 1988 Haldane proposed a spinless fermion model for IQHE without Landau levels, in which two independent effective Hamiltonian with the same form of 2D Dirac equation were obtained.<sup>11</sup> The Haldane model was generalized to the graphene lattice model of spin 1/2 electrons, which exhibits quantum spin Hall effect.<sup>12</sup> Bernevig, Hughes and Zhang predicted that QSHE can be realized in HgTe/CdTe quantum well and proposed an effective model,<sup>14</sup>

$$H_{\text{BHZ}} = \begin{pmatrix} h(k) & 0 \\ 0 & h^*(-k) \end{pmatrix}, \quad (42)$$

where  $h(k) = \epsilon(k) + A(k_x\sigma_x + k_y\sigma_y) + (M - Bk^2)\sigma_z$ . The model is actually equivalent to the 2D Dirac model as shown in Eq. (22), in addition to the kinetic term  $\epsilon(k)$ ,

$$h(k) = \epsilon(k) + h_+; h^*(-k) = \epsilon(k) + Uh_-U^{-1}, \quad (43)$$

where the unitary transformation matrix  $U = \sigma_z$ .

If the inclusion of  $\epsilon(k)$  does not close the energy gap caused by  $M$  for a non-zero  $B$ , there exists a topological phase transition from a positive  $M$  to a negative  $M$ . However, the sign of  $M$  alone cannot determine whether the system is topologically trivial or non-trivial. From the formula in Eq. (28), we know that the system is in the quantum spin Hall phase only for  $MB > 0$  and there exists a pair of helical edge states around the boundary of system. A general discussion can be found in the paper by Zhou *et al.*<sup>50</sup> Finally we want to comment on one popular opinion that the band inversion induces the topological quantum phase transition. If  $B = 0$ , the system is always topologically trivial for either positive or negative  $M$ , though there exists a bound state at the interface of two systems with positive and negative  $M$ , respectively.

The surface states of a thin film of topological insulator such as  $\text{Bi}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$  can be also described by a two-dimensional Dirac model.<sup>54, 53</sup> The mass or the band gap of the Dirac particles originates from the overlap of the wavefunctions of the top and bottom surface states. The gap opening of the two surface states was observed in  $\text{Bi}_2\text{Se}_3$  thin films experimentally,<sup>57, 58</sup> and was also confirmed numerically by the first-principle calculations<sup>59</sup>. Recently Luo and Zunger<sup>60</sup> reported a first-principle calculation for  $\text{HgTe}/\text{CdTe}$  quantum well and presented a different picture that the topological quantum phase transition occurs at the crossing point of two ‘‘interface-localized’’ states. This is in good agreement of the theory for 3D topological insulator thin films.<sup>61</sup>

### 6.3. Three-Dimensional Topological Insulators

The 3D Dirac equation can be applied to describe a large family of three-dimensional topological insulators.  $\text{Bi}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$  and  $\text{Sb}_2\text{Te}_3$  have been confirmed to be topological insulator with a single Dirac cone of surface states. For example, in  $\text{Bi}_2\text{Se}_3$ , the electrons near the Fermi surfaces mainly come from the  $p$ -orbitals of Bi and Se atoms. According to the point group symmetry of the crystal lattice,

$p_z$  orbital splits from  $p_{x,y}$  orbitals. Near the Fermi surface the energy levels turn out to be the  $p_z$  orbital. The four orbitals are used to construct the eigenstates of parity and the basis for the effective Hamiltonian,<sup>34</sup> which has the exact form as

$$H = \epsilon(k) + \sum_{i=x,y,z} v_i p_i \alpha_i + (mv^2 - \sum_{i=x,y,z} B_i p_i^2) \beta, \quad (44)$$

with  $v_x = v_y = v_{\parallel}$  and  $v_z = v_{\perp}$  and  $B_x = B_y = B_{\parallel}$  and  $B_z = B_{\perp}$ .  $\epsilon(k) = C - D_{\parallel}(p_x^2 + p_y^2) - D_{\perp}p_z^2$ . In this way the effective Hamiltonian in the  $x$ - $y$  plane has the form<sup>53</sup>

$$H_{\text{eff}} = \sqrt{1 - D_{\perp}^2/B_{\perp}^2} v_{\parallel} (p \times \sigma)_z, \quad (45)$$

or under a unitary transformation

$$H_{\text{eff}} = \sqrt{1 - D_{\perp}^2/B_{\perp}^2} v_{\parallel} (p_x \sigma_x + p_y \sigma_y). \quad (46)$$

We note that the inclusion of  $\epsilon(k)$  will revise the effective velocity of the surface states, which is different from the result in Ref. 34.

## 7. From the continuous model to the lattice model

In practice, the continuous model is sometimes mapped into a lattice model in the tight binding approximation. In a  $d$ -dimensional hyper-cubic lattice, one replaces<sup>62, 63</sup>

$$k_i \rightarrow \frac{1}{a} \sin k_i a, \quad (47)$$

$$k_i^2 \rightarrow \frac{2}{a^2} (1 - \cos k_i a), \quad (48)$$

which are equal to each other in a long wave limit. Usually there exists the fermion doubling problem in the lattice model for massless Dirac particles. The replacement of  $k_i \rightarrow \sin k_i a/a$  will cause an additional zero point at  $k_i a = \pi$  besides  $k_i a = 0$ . Thus there exist four Dirac cones in a square lattice at  $k = (0, 0)$ ,  $k = (0, \pi/a)$ ,  $k = (\pi/a, 0)$  and  $(\pi/a, \pi/a)$  for a gapless Dirac equation. A large  $B$  term removes the problem as  $2B(1 - \cos k_i a)/a^2 \rightarrow B/a^2$  in the lattice model. Thus the lattice model is equivalent to the continuous model only in the condition of a large  $B$ . The zero point of  $(1 - \cos k_i a)^2$  is at  $k_i a = \pi/2$  not 0 or  $\pi$  in  $\sin k_i a$ . Thus for a finite  $B$ , the band gap may not open at the  $\Gamma$  point in the lattice model because of the competition between the linear term and the quadratic term of  $k_i$ . This fact may lead to a topological transition from a large  $B$  to a small  $B$ . Imura *et al.*<sup>64</sup> analyzed the 2D case

in details and found that there exists a topological transition at a finite value of  $B$  in two dimensions. A similar transition will also exist in higher dimensions. One should be careful when studying the continuous model in a tight binding approximation.

## 8. Conclusion

To summarize, we found that the  $Z_2$  index for the Dirac equation is always zero, and thus the Dirac equation is topologically trivial. After the quadratic  $B$  term is introduced to correct the mass  $m$  of the Dirac equation, the  $Z_2$  index is modified as 1 for  $mB > 0$  and 0 for  $mB < 0$ . For a fixed  $B$  there exists a topological quantum phase transition from a topologically trivial system to a non-trivial system when the sign of mass  $m$  changes.

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

- in 1D, there exists the bound state of zero energy near the ends;
- in 2D, there exists the solution of helical edge states near the edges;
- in 3D, there exists the solution of the surface states near the surface;
- in higher dimension, there always exists the solution of higher dimension surface.

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

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