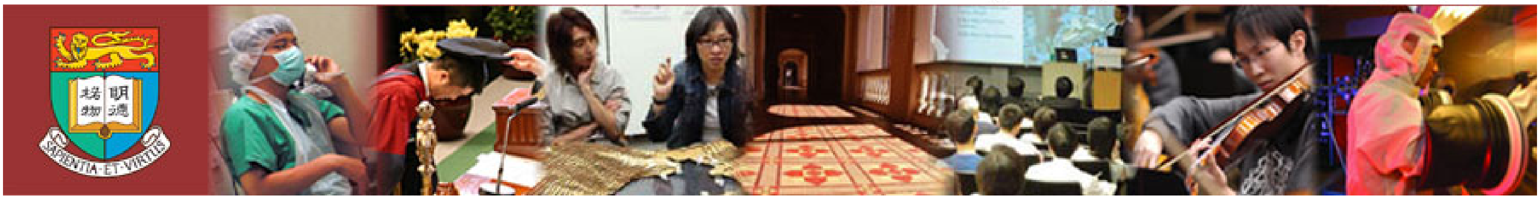

Title	TOPOLOGICAL INSULATOR AND THE DIRAC EQUATION
Author(s)	Shen, S; SHAN, W; Lu, H
Citation	SPIN, 2011, v. 1 n. 1, p. 33-44
Issued Date	2011
URL	http://hdl.handle.net/10722/242502
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TOPOLOGICAL INSULATOR AND THE DIRAC EQUATION

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(Dated: June 20, 2012)

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 B term in momentum is introduced to correct the mass term m or the band gap 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 one 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.

PACS numbers:

INTRODUCTION

Translational invariance in crystal lattices and the Bloch theorem for the wave function of electrons in solid make it possible for us to know the band structures of solid and why a solid is a metal, an insulator or semiconductor. Recent years it is found that a new class of materials possess 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 is called topological insulator.[1–3]

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.[4] 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 hetero-junction in a strong magnetic field, in which longitudinal conductance becomes zero while the quantum plateau of the Hall conductance appears at $\nu e^2/h$ (ν is an integer).[5] Two years later Tsui et al observed the fractional quantum Hall effect (FQHE) in a sample with higher mobility.[6] In the theory of edge states for IQHE electrons form discrete Landau levels in a strong magnetic field. Electrons in the bulk has 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.[7, 8] 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 to form stable metallic edge states.[9, 10] The quasi-particles in FQHE have fractionalized charges, and obeys new quantum statistics. In 1988 Haldane proposed that IQHE could be realized in a lattice system of spinless fermions in a period magnetic flux.[11] Though the total magnetic flux is zero, electrons are driven to form an conducting edge channel by the 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.[12] 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 an spin-dependent magnetic field to employ on electron spins. Different electron spins experience opposite spin-orbit force, i.e., spin transverse force.[13] As a result, a bilayer Haldane model may be realized in a spin-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: 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 channel is prohibited due to the symmetry. Bernevig, Hughes and Zhang predicted that the QSHE effect can be realized in the HgTe/CdTe sandwiched quantum well.[14] 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.[15, 16] This prediction was confirmed experimentally by Konig et al soon after the prediction.[17] The stability of the QSHE was studied by several groups.[18–21] 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 an conducting helical edge channels appear.[22] This phase was studied numerically and analytically.[23, 24] Strong Coulomb interactions may also generate QSHE in Mott insulators.[25, 26]

The generalization of QSHE to three dimension is topologically non-trivial.[27–30] Kane and Mele proposed a Z_2 index to classify the materials with time reversal invariance into a strong and weak topological insulator.[31] 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 are prohibited because of the symmetry. $Bi_{1-x}Sb_x$ was predicted to be 3D topological insulator by Fu and Kane[32] and was verified experimentally.[33] Zhang et al [34] and Xia et al[35] pointed out that Bi_2Te_3 and Bi_2Se_3 are topological insulator with a single Dirac cone of the surface states. ARPES data showed clearly the existence of single Dirac cone in Bi_2Se_3 [35] and Bi_2Te_3 [36]. 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. [37]proposed the unconventional magneto-electric 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 eqautions. It is regarded as one of the characteristic features of the topological insulators [38, 39]. Fu and Kane proposed a possible realization of Majorana fermions as an proximity effect of s-wave superconductor and surface states of topological insulator.[40] The Majorana fermions are topologically protected from local sources of decoherence, and will be of potential application in universal quantum computor.[41, 42] 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 wave function for elementary spin 1/2 particle.[43, 44] It enters the field of topological insulator in two aspects. First of all, topological insulators possess strong spin-orbit coupling, which is a consequence of the Dirac equation.[45] It makes the spin, momentum and the Coulomb interaction or external electric fields couple together. As a result it is possible that the band structures in some materials becomes topologically non-trivial. Another aspect is that the effective Hamiltonians to the QSHE and 3D topological insulators have the identical mathematical structure of the Dirac equation. In these effective models the equations are used to describe the coupling between electrons the conduction and valence bands, not the electron and positions in Dirac's theory. The positive and negative spectra are for the electrons and hole in semiconductors not in the high energy physics. The conventional Dirac equation is time-reversal invariant. For a system with time reversal symmetry, the effective Hamiltonian to describe the electrons near the Fermi level can be derived from the theory of invariants. As a result of the $k \cdot p$ expansion of the band structure, some effective continuous models have the same form of the Dirac equation.

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.

DIRAC EQUATION AND SOLUTIONS OF THE BOUND STATES

In 1928, Paul A. M. Dirac wrote down an equation for relativistic quantum mechanical wave functions, which describes elementary spin-1/2 particles,[43, 44]

$$H = cp \cdot \alpha + mc^2 \beta \tag{1}$$

where m is the rest mass of particle and c is the speed of light. α_i and β are the Dirac matrices satisfying

$$\alpha_i^2 = \beta^2 = 1 \tag{2a}$$
$$\alpha_i \alpha_j = -\alpha_j \alpha_i \tag{2b}$$
$$\alpha_i \beta = -\beta \alpha_i \tag{2c}$$

In 2D spatial space, the Dirac matrices have the same forms of the Pauli matrices σ_i, i.e., $\alpha_x = \sigma_x$, $\alpha_y = \sigma_y$, and $\beta = \sigma_z$. In three dimensional spatial space, one representation of the Dirac matrices in terms of the Pauli matrices σ_i $(i = x, y, z)$ is

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \tag{3a}$$

$$\beta = \begin{pmatrix} \sigma_0 & 0 \\ 0 & -\sigma_0 \end{pmatrix} \tag{3b}$$

where σ_0 is a 2×2 identity matrix. From this equation, the 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 predates the discovery of position, the antiparticle of the electron. It is one of the main achievements of modern theoretical physics.

Under the transformation of $m \to -m$ it is found that the equation remains invariant if $\beta \to -\beta$, which satisfies all mutual anticommutation relations for α_i and β. 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

$$h(x) = -iv\hbar\partial_x \sigma_x + m(x)v^2 \sigma_z \tag{4}$$

and

$$m(x)=\begin{cases}-m_1 & \text{if} \quad x<0\\ +m_2 & \text{otherwise}\end{cases} \tag{5}$$

(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

$$\Psi(x)=\sqrt{\frac{v}{\hbar}\frac{m_1m_2}{m_1+m_2}}\begin{pmatrix} i\\ 1\end{pmatrix}e^{-|m(x)vx|/\hbar}. \tag{6}$$

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 fractionalized charge in one-dimensional system.[46]. 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 does not vanish at the interface when $m_2\to+\infty$. 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 which the wave functions dominantly distributes around the interface. One solution has the form

$$\Psi(x,k_y)=\sqrt{\frac{v}{h}\frac{m_1m_2}{m_1+m_2}}\begin{pmatrix} i\\ 0\\ 0\\ 1\end{pmatrix}e^{-|m(x)vx|/\hbar+ik_yy} \tag{7}$$

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

$$\Psi(x,k_y)=\sqrt{\frac{v}{h}\frac{m_1m_2}{m_1+m_2}}\begin{pmatrix} 0\\ i\\ 1\\ 0\end{pmatrix}e^{-|m(x)vx|/\hbar+ik_yy} \tag{8}$$

with the dispersion $\epsilon_k=-v\hbar k_y$. Both states carry a current along the interface, but electrons moving in opposite directions. The currents decays 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 are $\epsilon_p=\pm vp$. 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.

MODIFIED DIRAC EQUATION AND Z2 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,

$$H=v\mathbf{p}\cdot\alpha+\left(mv^2-B\mathbf{p}^2\right)\beta. \tag{9}$$

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 wave functions can be expressed as $\Psi_\nu=u_v(p)e^{i(p\cdot r-E_{p,\nu}t)/\hbar}$. 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 $u_v(p)$ can be expressed as $u_v(p)=Su_\nu(p=0)$ with

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

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

The topological properties of the modified Dirac equation can be gained from these solutions of a free particle. The Dirac equation is invariant under the time-reversal symmetry, and can be classified according to the Z_2 topological classification following Kane and Mele.[31]. In the representation for the Dirac matrices in Eq. (**??**), the time-reversal operator here is defined as[47] $\Theta\equiv -i\alpha_x\alpha_z\mathcal{K}$, where $\mathcal{K}$ the complex conjugate operator that forms the complex conjugate of any coefficient that multiplies a ket or wave function (and stands on the right of $\mathcal{K}$). Under the time reversal operation, the modified Dirac equation remains invariant, $\Theta H(p)\Theta^{-1}=H(-p)$ (p is a good quantum number of the momentum). Furthermore we have the relations that $\Theta u_1(p)=-iu_2(-p)$ and $\Theta u_2(p)=+iu_1(-p)$, which satisfy the relation of $\Theta^2=-1$. 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

$$\begin{pmatrix} 0 & i\frac{mv^2-Bp^2}{E_{p,1}} & -i\frac{p_-v}{E_{p,1}} & i\frac{p_zv}{E_{p,1}}\\ -i\frac{mv^2-Bp^2}{E_{p,1}} & 0 & i\frac{p_zv}{E_{p,1}} & i\frac{p_+v}{E_{p,1}}\\ i\frac{p_-v}{E_{p,1}} & -i\frac{p_zv}{E_{p,1}} & 0 & i\frac{mv^2-Bp^2}{E_{p,1}}\\ -i\frac{p_zv}{E_{p,1}} & -i\frac{p_+v}{E_{p,1}} & -i\frac{mv^2-Bp^2}{E_{p,1}} & 0\end{pmatrix}. \tag{11}$$

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

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

which is the Pfaffian for the 2×2 matrix. According to Kane and Mele,[31] the even or odd number 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 $mB \le 0$ and there exists no zero in the Pfaffian, we conclude immediately that the modified Dirac Hamiltonian for $mB \le 0$ including the conventional Dirac Hamiltonian ($B = 0$) is topologically trivial.

For $mB > 0$ the case is different. In this continuous model, the Brillouin zone becomes infinite. At $p = 0$ and $p = +\infty$, $P(0) = i\mathrm{sgn}(m)$ and $P(+\infty) = -i\mathrm{sgn}(B)$. 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 $a \to 0$ and the reciprocal lattice vector $G = 2\pi/a \to +\infty$. In this sense as a limit of a square lattice other three TRIM 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 TRIM have opposite sign of $P(0)$. Following Fu, Kane and Mele[27, 32], we conclude that *the modified Dirac Hamiltonian is topologically non-trivial only if* $mB > 0$.

In two dimension Z_2 index can be determined by evaluating the winding number of the phase of $P(p)$ around a loop of enclosing the half the Brilouin zone in the complex plane of $\mathbf{p} = p_x + ip_y$,

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

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

TOPOLOGICAL INVARIANTS AND QUANTUM PHASE TRANSITION

An alternative approach to explore the topological property of the Dirac model is the Green function method.[48] Volovik [49]proposed that the Green function rather than the Hamiltonian is more applicable to classify the topological insulator. From the Dirac equation, the Green function has the form

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

where $h^2(k) = H^2 = v^2p^2 + (mv^2 - Bp^2)^2$. There is the following topological invariant

$$\tilde{N} = \frac{1}{24\pi^2}\epsilon_{ijk}\mathrm{Tr}[K_{i\omega_n=0}d\mathbf{p}G\partial_{p_i}G^{-1}G\partial_{p_j}G^{-1}G\partial_{p_k}G^{-1}]$$

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

$$\tilde{N} = \mathrm{sgn}(m) + \mathrm{sgn}(B).$$

When $mB > 0$, $\tilde{N} = \pm 2$, which define the phase topologically non-trivial. If B is fixed to be positive, there exist a quantum phase transition from topologically trivial phase of $m < 0$ to a topologically non-trivial phase. This is in a good agreement with the result of Z2 index in the preceding section.

Except for the phases of $\tilde{N} = \pm 2$, it is found that there exist a marginal topological phases of $\tilde{N} = \pm 1$. For free Dirac fermions of $B = 0$, the topological invariant $\tilde{N} = sgn(m)$. It is +1 for a positive mass and -1 for a negative mass. Their difference $\Delta\tilde{N} = 2$ 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 II. There exists an intermediate gapless phases of $m = 0$ between two 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 as the free Dirac fermions.

THE TOPOLOGICALLY PROTECTED BOUNDARY STATES SOLUTIONS

1D: the bound state of zero energy

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

$$h(x) = vp_x\sigma_x + \left(mv^2 - Bp_x^2\right)\sigma_z. \quad (14)$$

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 wave function vanishes at $x = +\infty$. In the condition of $mB > 0$, there exists a solution of the bound state with zero energy

$$\begin{pmatrix}\varphi\\ \chi\end{pmatrix} = \frac{C}{\sqrt{2}}\begin{pmatrix}\mathrm{sgn}(B)\\ i\end{pmatrix}\left(e^{-x/\xi_+} - e^{-x/\xi_-}\right) \quad (15)$$

$$\xi_{\pm}^{-1} = \frac{v}{2\left|B\right|\hbar}\left(1 \pm \sqrt{1-4mB}\right) \tag{16}$$

where C is the normalization constant. The main feature of this solution is that the wave function dominantly distributes near the boundary. The two parameters $\xi_- > \xi_+$ and decides the spatial distribution of the wave function. This is a very important length scale, which characterizes the bound state. 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. 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 the conventional Dirac equation. In this sense, the two equations reach at the same conclusion.

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

$$\Psi_1 = \frac{C}{\sqrt{2}}\begin{pmatrix} \mathrm{sgn}(B) \\ 0 \\ 0 \\ i \end{pmatrix}(e^{-x/\xi_+} - e^{-x/\xi_-}) \tag{17a}$$

$$\Psi_2 = \frac{C}{\sqrt{2}}\begin{pmatrix} 0 \\ \mathrm{sgn}(B) \\ i \\ 0 \end{pmatrix}(e^{-x/\xi_+} - e^{-x/\xi_-}) \tag{17b}$$

2D: the helical edge states

In two dimension, the equation is decoupled into two independent equations

$$h_{\pm} = vp_x\sigma_x \pm vp_y\sigma_y + \left(mv^2 - Bp^2\right)\sigma_z. \tag{18}$$

These two subsets of equations breaks the "time" reversal symmetry under the transformation of $\sigma_i \to -\sigma_i$ and $p_i \to -p_i$.

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

$$H_{eff} = (\langle\Psi_1|, \langle\Psi_2|)\Delta H\begin{pmatrix} |\Psi_1\rangle \\ |\Psi_2\rangle \end{pmatrix} = vp_y\mathrm{sgn}(B)\sigma_z \tag{19}$$

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

$$\epsilon_p = \pm vp_y \tag{20}$$

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

The exact solutions of the edge states to this 2D equation have the similar form of 1D[50]

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

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

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

$$\xi_{\pm}^{-1} = \frac{v}{2\left|B\right|\hbar}\left(1 \pm \sqrt{1-4mB+4B^2p_y^2/v^2}\right). \tag{22}$$

In two-dimension, the Chern number or Thouless-Kohmoto-Nightingale-Nijs integer can be used to characterize whether the system is topologically trivial or nontrivial.[51] Write the Hamiltonian in Eq. (18) in the form $H = \mathbf{d}(p)\cdot\sigma$ The Chern number is expressed as

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

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

$$n_{\pm} = \pm(\mathrm{sgn}(m) + \mathrm{sgn}(B))/2. \tag{23}$$

which gives the Hall conductance $\sigma_{\pm} = n_{\pm}e^2/h$. When m and B have the same sign, $n_{\pm}$ becomes ± 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 relation of integer quantum Hall effect.[55]

3D: the surface states

In 3D, we consider an 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 $H_{1D}(x)$,

$$\Delta H_{3D} = vp_y\alpha_y + vp_z\alpha_z - B(p_y^2 + p_z^2)\beta. \tag{24}$$

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

$$H_{eff} = (\langle\Psi_1|, \langle\Psi_2|)\Delta H_{3D} \begin{pmatrix} |\Psi_1\rangle \\ |\Psi_2\rangle \end{pmatrix} = v\text{sgn}(B)(p \times \sigma)_x. \quad (25)$$

Under a unitary transformation,

$$\Phi_1 = \frac{1}{\sqrt{2}}(|\Psi_1\rangle - i|\Psi_2\rangle) \quad (26a)$$

$$\Phi_2 = \frac{-i}{\sqrt{2}}(|\Psi_1\rangle + i|\Psi_2\rangle) \quad (26b)$$

we can have a gapless Dirac equation for the surface states

$$\begin{aligned} H_{eff} &= \frac{1}{2}(\langle\Phi_1|, \langle\Phi_2|)\Delta H_{3D} \begin{pmatrix} |\Phi_1\rangle \\ |\Phi_2\rangle \end{pmatrix} \\ &= v\text{sgn}(B)(p_y\sigma_y + p_z\sigma_z). \end{aligned} \quad (27)$$

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

$$\Psi_\pm = C\Psi_\pm^0(e^{-x/\xi_+} - e^{-x/\xi_-})\exp[+i\,(p_y y + p_z z)\,/\hbar] \quad (28a)$$

where

$$\Psi_+^0 = \begin{pmatrix} \cos\frac{\theta}{2}\text{sgn}(B) \\ -i\sin\frac{\theta}{2}\text{sgn}(B) \\ \sin\frac{\theta}{2} \\ i\cos\frac{\theta}{2} \end{pmatrix} \quad (28b)$$

$$\Psi_-^0 = \begin{pmatrix} \sin\frac{\theta}{2}\text{sgn}(B) \\ i\cos\frac{\theta}{2}\text{sgn}(B) \\ -\cos\frac{\theta}{2} \\ i\sin\frac{\theta}{2} \end{pmatrix} \quad (28c)$$

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

$$\xi_\pm^{-1} = \frac{v}{2|B|\hbar}\left(1 \pm \sqrt{1 - 4mB + 4B^2p^2/\hbar^2}\right). \quad (29)$$

Generalization to higher dimensional topological insulators

The solution can be generalized to higher dimensional system. We conclude that there always exists a d-dimensional surface state in the modified Dirac equation.

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 or others 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,

$$H = \epsilon(p_i) + \sum_i v_i p_i \alpha_i + (mv^2 - \sum_i B_i p_i^2)\beta. \quad (30)$$

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 k·p theory as an expansion of the momentum p near the Γ point. Since under the time reversal, $\beta \to \beta$ and $\alpha \to -\alpha$, if we expand an time reversal invariant Hamiltonian near the Γ point, the zero-order term should be constant, $\epsilon(0)$ and $mv^2\beta$. The first order term in the momentum must $\sum_i v_i p_i \alpha_i$ since $p_i \to -p_i$ under time reversal. 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 α. The summation up to the second order terms give the modified Dirac equation.

Complex p-wave spinless superconductor

A complex p-wave spinless superconductor has two topologically distinct phases, one is the strong pairing phase and another is the weak pairing phase.[48, 56] The weak pairing phase is identical to the Moore-Read quantum Hall state.[56] 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

$$K_{eff} = \sum_k \left[\xi_k c_k^\dagger c_k + \frac{1}{2}(\Delta_k^* c_{-k} c_k + \Delta_k c_k^\dagger c_{-k}^\dagger)\right]. \quad (31)$$

The normalized ground state has the form

$$|\Omega\rangle = \prod_k (u_k + v_k c_k^\dagger c_{-k}^\dagger)|0\rangle. \quad (32)$$

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

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_k \\ v_k \end{pmatrix} = \begin{pmatrix} \xi_k & -\Delta_k^* \\ -\Delta_k & -\xi_k \end{pmatrix}\begin{pmatrix} u_k \\ v_k \end{pmatrix} \quad (33)$$

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

$$\Delta_k = \Delta(k_x - ik_y); \xi_k = \frac{k^2}{2m} - \mu \tag{34}$$

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

$$H_{eff} = -\Delta\left(k_x\sigma_x + k_y\sigma_y\right) + \left(\frac{k^2}{2m} - \mu\right)\sigma_z \tag{35}$$

The Chern number of the effective Hamiltonian becomes

$$n = \left[\mathrm{sgn}(\mu) + \mathrm{sgn}(1/m)\right]/2 \tag{36}$$

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 μ the Chern number is 0. For $\mu = 0$, the Chern number is equal to one half, which is similar to the case of $m \to +\infty$ and a finite μ. If the quadratic term in ξ_k is neglected, we see that the topological property will change completely.

Usually for a positive μ, the system is in a weak pairing phase, for a negative μ the strong coupling phase. Including the quadratic term in ξ_k we conclude that the weak pairing phase for positive μ 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.[50] Read and Green[56] 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 and 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 as a 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.[40] The state support Majorana bound states at vortices.

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 the Dirac equation were obtained.[11] The Haldane's model was generalized to the graphene lattice model of spin 1/2 electrons, which exhibits quantum spin Hall effect.[12] Bernevig, Hughes and Zhang predicted that QSHE can be realized in HgTe/CdTe quantum well and proposed an effective model,[14]

$$H_{BHZ} = \begin{pmatrix} h(k) & 0 \\ 0 & h^*(-k) \end{pmatrix} \tag{37}$$

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.(18) in addition of the kinetic term $\epsilon(k)$,

$$h(k) = \epsilon(k) + h_+; h^*(-k) = \epsilon(k) + Uh_-U^{-1}, \tag{38}$$

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.(23), we know that the system is in a 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.[50] 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 Bi_2Te_3 and Bi_2Se_3 can be also described by a two-dimensional Dirac model.[53, 54] The mass or the band gap of the Dirac particles originates from the overlapping of the wave functions of the top and bottom surface states. The gap opening of the two surface states were observed in Bi_2Se_3 thin films experimentally[57, 58], and was also confirmed numerically by DFT[59]. Recently Luo and Zunger [60] reported a DFT calculation for HgTe/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 a good agreement of the theory for 3D topological insulator thin film.[61]

Three-Dimensional Topological Insulators

The 3D Dirac equation can be applied to describe a large family of three-dimensional topological insulators. Bi_2Te_3 and Bi_2Se_3 and Sb_2Te_3 have been confirmed to be topological insulator with a single Dirac come of surface states. For example, in Bi_2Te_3, the electrons near the Fermi surfaces mainly come from the p-orbitals of Bi and Te atoms. According to the point group symmetry of the crystal lattice, p_z orbital splits from $p_{x,y}$ orbital. 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 base for the effective Hamiltonian,[34] which has the exact form as

$$H = \epsilon(k) + \sum_{i=x,y,z} v_i p_i \alpha_i + (mv^2 - \sum_{i=x,y,z} B_i p_i^2)\beta. \quad (39)$$

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

$$H_{eff} = \sqrt{1 - D_\perp^2/B_\perp^2} v_{\shortparallel} (p \times \sigma)_z \quad (40)$$

or under a unitary transformation

$$H_{eff} = \sqrt{1 - D_\perp^2/B_\perp^2} v_{\shortparallel} (p_x\sigma_x + p_y\sigma_y). \quad (41)$$

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].

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[62, 63]

$$k_i \rightarrow \frac{1}{a}\sin k_i a \quad (42)$$
$$k_i^2 \rightarrow \frac{2}{a^2}(1 - \cos k_i a) \quad (43)$$

which are equal to each other in a long wave limit. Usually there exits 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 two Dirac cones in a square lattice at $k = (0, 0)$ 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 π in $\sin k_i a$. Thus for a finite B, the band gap may not open at the Γ 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 [64] analyzed the 2D case in details and found that there exists a topological transition at a finite value of B in two-dimension. A similar transition will also exist in higher dimension. It should be careful when we study the continuous model in a tight binding approximation.

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 one 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 boundary;
- in 2D, there exists the solution of helical edge states near the boundary;
- 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 families of topological insulators from one to higher dimension.

Acknowledgements
This work was supported by the Research Grant Council of Hong Kong under Grant No. HKU7051/10P and HKUST3/CRF/09.

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