The theoretical development and prospect of two-dimensional topological insulators

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Abstract. Topological insulators can be described as rediscovery of band theory, where numerous secrets on edges and surfaces are unearthed. During the process of rediscovery, the concept of topology into novel theoretical models of topological insulators played a crucial role. This paper aims to give an introduction to the theoretical development of two-dimensional topological insulators in a nutshell, so it is indispensable and efficient to relate topological invariant with the band structure of topological insulators and use specific and vital theoretical models to reveal novel phenomena in those materials. The main focus of the paper is placed on historic landmarks in the theoretical development of two-dimensional topological insulators where fundamental concepts and models have paved the way for further enrichment of family of topological materials and experimental realizations.

1. Introduction
Over the past decades, topological insulator has drawn extensive concern in condensed matter physics due to its unique electronic behavior on its edges (2D) or surfaces (3D). Distinguished from common insulators, conductors and semiconductors, topological insulators (TIs) are insulated inside but have metallic states outside and the most exhilarating characteristic is the topology part of them, which dispels the influence of continuous deformation that does not break the underlying symmetry. Such robustness against continuous deformation is underpinned by two cornerstones. The first is the time reversal symmetry (TRS) where the Hamiltonian function keeps unchanged, while momentum and spin reverse their directions and the other is the spin-orbit coupling (SOC) aspect of TIs. The SOC acts like a magnetic field and induces band overlapping to achieve edge/surface states in TIs. At the beginning of this paper, theoretical development of 2D topological insulators is reviewed in Section 2 by setting out from some basic concepts and the calculation of Hall conductivity. Then in section 3, important theoretical models of 2D TIs are introduced. Finally, conclusions and outlooks are given in section 4.

2. Berry phase, the TKNN invariant and Hall conductivity
One essential question about topological insulator is that why topological insulator having metallic edges/surfaces states is termed as ‘topological’. A limpid illustration of topology using common objects is given by considering the relation between a donut and a coffee cup. Imagine that the donut is made of some sort of pliable materials so that one could shape the left half part into a cylinder continuously with the right half donut sticking to the cylinder. Then press the top of the cylinder until the sag is deep enough. In this way, one could smoothly deform a donut into a coffee cup and vice versa, so it can be claimed that these two objects are topologically equivalent. Actually, it is the
winding number of objects that defines their topological equivalence. For example, a sphere with a
different winding number cannot be smoothly reshaped into a coffee cup or a donut unless you cut and
open a hole in it. Analogical to this pattern, electronic band dispersion in condensed matter systems
also have such topological classification by defining appropriate topological invariant, while the object
cited to calculate topological invariant is the wave function of electron instead of being the
configuration of objects in real space. In order to identify topologically nontrivial systems, the concept
of Berry phase is borrowed as demonstrated below.

Berry phase delineates the adiabatic evolution of a quantum state and can be used to understand
the TKNN invariant which identifies the topology of a system. By considering parameter vectors evolving
with time slowly enough to describe quantum states and splitting the phase expression into the
dynamic phase and the Berry phase, the primitive form of Berry phase is defined in the following
form

\[ \gamma_s(C) = \frac{i}{\hbar} \oint_C \langle n(R) | \nabla_R n(R) \rangle \cdot dR \]  

where \( R \) is time-dependent and represents a path in the parameter space.

When considering a concrete model of the Chern insulator introduced by Haldane[2], the parameter
space becomes the wave vector space and the quantum state is a bulk state \( |\psi\rangle \) related to the wave
vector \( k \) and spin \( s \). Then defining a vector-potential

\[ A_{k,s} = i \langle \psi_{k,s} | \frac{\partial}{\partial k} \psi_{k,s} \rangle \]  

and using the Stoke’s theorem, the Berry phase can be written in the following form

\[ \gamma_s = \int (\nabla_k \times A_{k,s}) \cdot d\kappa_{x,y} \]  

In order to illustrate the connection between Berry phase integral and the Hall conductivity, an
observable quantity revealing topological characteristics of a system, the TKNN formula[3] shall be
introduced here. In a two dimensional conductor, the Kubo formula calculating Hall conductivity is
written as

\[ \sigma_{xy} = \frac{ie^2}{\hbar A_j} \sum_{\epsilon_\alpha < \epsilon_\beta} \left( \frac{\partial H}{\partial k_x} \right)_{\alpha\beta} \left( \frac{\partial H}{\partial k_y} \right)_{\beta\alpha} \left( \frac{\partial H}{\partial k_y} \right)_{\alpha\beta} \left( \frac{\partial H}{\partial k_x} \right)_{\beta\alpha} \]  

where \( A_j \) is the area of the system, \( \epsilon_\alpha, \epsilon_\beta \) are eigenvalues of the Hamiltonian \( \hat{H} \) and \( E_F \) is the
Fermi level.

Through some basic quantum mechanical calculation, replacing the summation of \( \epsilon_\beta \) with the
summation of \( \epsilon_\alpha \) and choosing appropriate boundary conditions, the expression for the quantum
Hall conductivity in transverse direction can be obtained as:

\[ \sigma_{xy} = \frac{ie^2}{\hbar A_j} \sum_{\epsilon_\alpha < \epsilon_F} \left( \partial_{k_x} \alpha \partial_{k_y} \alpha - \partial_{k_y} \alpha \partial_{k_x} \alpha \right) \]  

As is known, when using Kubo formula to calculate conductivity, we only concern about the
occupied states, so it is crucial to exclude the contribution of unoccupied states in the process. Then
for occupied states, define the vector-potential in the following way

\[ A_{k,j} = i \sum_{\epsilon_\alpha < \epsilon_F} \langle \alpha | \partial_j | \alpha \rangle \]  

where \( j \) represents x or y direction. From here, the linkage between the integral of Berry curvature
over the filled states and the Hall conductivity has been established. The TKNN formula for a two
dimensional system can be obtained from the definition in Equation (6):

\[ \sigma_{xy} = \frac{e^2}{2\pi\hbar} \int (\nabla_k \times A_k) \cdot d\kappa_x d\kappa_y \]
Noting that Equation (7) and (3) have similar expression, it is easy to find out mathematical correspondence between the quantum Hall conductivity and the Berry phase curvature. To show the integer characteristic of the Hall conductivity, a transformation shall be exerted on the Brillouin zone (choosing it to be a rectangular for convenience) and consequently, the Brillouin zone is shaped into a torus which has no boundary (see Figure 1)[4], thus the domain of integration can be shifted from the whole Brillouin zone (BZ) to the curve C. With curve

\[ C \]

Figure 1. Topologically equivalent transformation of Brillouin zone

C on the right side of area I and on the left side of area II, two parts of the integral have opposite signs. Using the gauge dependent property of vector potential \( \mathbf{A}_{\mathbf{k},s} \), which is

\[ \mathbf{A}_{\mathbf{k},s} \rightarrow \mathbf{A}_{\mathbf{k},s} - \frac{\partial \zeta(\mathbf{k})}{\partial \mathbf{k}} , \]

we have:

\[ \int_{C} \mathbf{A} \cdot \mathbf{\nabla} = \frac{e^2}{\hbar} \frac{1}{2\pi} \oint_{C} \mathbf{V}_{\mathbf{k}} \zeta \cdot d\mathbf{k} \]  

(8)

The function \( \zeta(\mathbf{k}(t)) \) must satisfy the condition that after a closed path, the final value of it and the initial value of it have a difference of the integral multiples of \( \frac{\pi}{2} \). As a result, the right side of Equation (7) is integral multiples of \( \frac{e^2}{\hbar} \) and the integer \( n \), where

\[ n = \frac{1}{2\pi} \int (\mathbf{V}_{\mathbf{k}} \times \mathbf{A}_{\mathbf{k}})_{z} dk_{x}dk_{y} \]  

(9)

is the TKNN invariant, also termed as the first Chern number.

On the contrary, for topologically trivial situation, if the Berry potential \( \mathbf{A}_{\mathbf{k}} \) is well chosen, the integral over the whole BZ would be zero and the Hall conductance vanishes. So the nonzero Hall conductivity here implies that for topologically nontrivial situation, special singularities must exist in the BZ so that continuous and single-valued gauge selection becomes impossible in a whole BZ.

Conventionally, quantum Hall edge states in 2D systems with a chiral flow along its 1D boundary exhibit such quantized Hall conductivity under the existence of a magnetic field. However, as shown below, Haldane demonstrated that even without net flux of external magnetic field, the 2D hexagonal model could still harbor nonzero Chern number, i.e., topological nontrivial state.

3. Two-dimensional topological insulators

3.1 Haldane model

In 1988, Haldane introduced a “2D graphite” model[2] with zero external magnetic field where integer Hall conductance arose due to breaking of time reversal invariance (TRI). The diagram of the honeycomb lattice model is shown in Figure 2.
Figure 2. Dots with different colors represent different sub-lattice sites. Black arrows show the directions of positive phase hopping in the state with broken TRI.

The black and white dots have opposite on-site energy. By adding a periodic magnetic flux density, magnetic flux $\phi_a$ in area $a$ and magnetic flux $\phi_b$ in area $b$ satisfy the condition that $\phi_a = -\phi_b$[5], so the total magnetic flux through a unit cell becomes zero, which leads to the consequence that apparently, hopping term $t_1$ between nearest sites remains unchanged, while hopping term $t_2$ between second nearest sites is changed due to additional phase term. Setting $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ to be the displacement from a white dot to its three nearest black dots and defining that $\mathbf{b}_1 = \mathbf{a}_2 - \mathbf{a}_3$, $\mathbf{b}_2 = \mathbf{a}_3 - \mathbf{a}_1$, and $\mathbf{b}_3 = \mathbf{a}_1 - \mathbf{a}_2$, we can express the Hamiltonian of the system in the following way

$$H(k) = 2t_2 \cos \left( \sum_{i=1,2,3} \cos (k \cdot \mathbf{b}_i) \right) + t_1 \left[ \sum_{i=1,2} \left[ \cos (k \cdot \mathbf{a}_i) \sigma_x + \sin (k \cdot \mathbf{a}_i) \sigma_y \right] + \sum_{i=1,2,3} \left[ M - 2t_2 \sin \left( \sum_{i=1,2,3} \sin (k \cdot \mathbf{b}_i) \right) \right] \sigma_z \right]$$

(10)

where $\sigma_{x,y,z}$ are Pauli matrices, $\phi$ is the phase term for $t_2$ and $M$ is the positive on-site energy.

By expanding the Hamiltonian in a linear way that $\mathbf{0} = \mathbf{k} - \mathbf{k}_0$ at two distinct corner zones $\mathbf{k}_0$ that is defined as $\mathbf{k}_0 \cdot \mathbf{b}_i = 0$ (having assumed that $|t_2 / t_1| < 1 / 3$, which excludes the possibility of bands overlapping), we can express the Hamiltonian of the effective models near the two points as

$$H_\pm = \frac{3t_1 a}{\hbar} (\mathbf{\hat{0}}_x \sigma_x - \mathbf{\hat{0}}_y \sigma_y) + m_\pm \left[ \frac{3t_1 a}{\hbar} \right]^2 \sigma_z$$

(11)

where $m_\pm = \pm M - 3\sqrt{3}t_2 \sin \phi$. Obviously, the $M$ term in the Hamiltonian opens a $+M$ and a $-M$ energy gap at two $\mathbf{k}_0$ points, respectively. Also we note that it is the $m_\pm$ term that breaks the TRS of the system. The Chern number of the model was calculated by Haldane using the Strëda formula[6] and the expression was

$$n = \frac{1}{2} \left[ \text{sgn}(m_+) + \text{sgn}(m_-) \right]$$

(12)

As a result, the Chern number can be $\pm 1$ or 0. The nonzero Chern numbers happen when $|M / t_2| < 3\sqrt{3} |\sin \phi|$ with finite energy gap between two bands remained.

Haldane model has proved to be quite impossible in experimental realization. However, it is interesting that realization of Haldane model has been achieved in recent research[7] by using ultra-cold fermions where TRS and inversion symmetry of the system was broken.

3.2 Kane and Mele Model and $Z_2$ Invariant

In 2005, based on Haldane’s graphene model, Kane and Mele[8] proposed a quantum spin Hall (QSH) system where spin of electron was taken into account and spin-orbit coupling (SOC) which locked the relative direction between spin and momentum of electron played a crucial role in deriving the helical edge state of the QSH system. In Kane and Mele model, no more magnetic flux exists to break TRS and the two edge states carrying spin currents of electrons are preserved by the TRS. This model, in the absence of a conservation of spin current, is more realistic and assumed to be stable under low
temperature. A schematic illustration of the transport behavior of a QSH system versus a QHE system is shown below in order to visualize their spin and momentum configuration.

![Figure 3. Electronic transport behavior in a quantum Hall insulator (left) and a QSH insulator (right).](image)

The direction of spin is locked to the momentum of electron. The spin direction of the red current is out of the plane, while the spin direction of the blue counterpart is into the plane.

The Hamiltonian of the Kane and Mele model can be written in the form that

\[
H = t \sum_{\langle ij \rangle} c_i^\dagger c_j + i\lambda_{SO} \sum_{\langle ij \rangle} v_{ij} c_i^\dagger s^z c_j + \sum_{\langle ij \rangle} i\lambda_R c_i^\dagger \left(s \times \hat{d}_{ij}\right) c_j + \sum_i \xi_i c_i^\dagger c_i
\]  

(13)

The fermion operator in the first term contains the spin index and \(t\) is the nearest hopping coefficient. The second term is the SOC term where \(v_{ij} = 2/\sqrt{3}(\hat{d}_1 \times \hat{d}_2)_z = \pm 1\) and \(\hat{d}_1\) and \(\hat{d}_2\) are unit vectors along the two bonds the electron traverses going from site \(j\) to \(i\). \(s^z\) is a Pauli matrix operating on the spin space of electron. The third term and the last term are nearest neighbor Rashba term and sublattice potential \((\xi_i = \pm 1)\), respectively.

After diagonalization, the Hamiltonian of the system is a four-band one and the Bloch wave function is a four-component spinor, thus the Bloch Hamiltonian must have 16 components. The 16 components consist of the identity matrix, 5 Dirac matrices \(\Gamma^a(a=1, 2, 3, 4, 5)\) and 10 commutators. The 5 Dirac matrices are even under time-reversal operator, while the 10 commutators are odd. The Hamiltonian can be expressed in Dirac matrices representation as

\[
H(k) = \sum_{a=1}^{5} d_a(k) \Gamma^a + \sum_{a,b} d_{ab}(k) \Gamma^{ab}
\]  

(14)

The corresponding nonzero coefficients are shown in Table 1 with \(x = k_x a / 2\) and \(\sqrt{3}k_y a / 2\), where \(\lambda_{SO}, \lambda_R, \lambda_v\) are coefficients of SOC term, Rashba term and sublattice potential term, respectively.

| Coefficient | Expression | Coefficient | Expression |
|-------------|------------|-------------|------------|
| \(d_1\)     | \(t(1 + 2\cos x \cos y)\) | \(d_{12}\)  | \(-2t\cos x \sin y\) |
| \(d_2\)     | \(\lambda_v\)            | \(d_{15}\)  | \(\lambda_{SO} (2\sin 2x - 4\sin x \cos y)\) |
| \(d_3\)     | \(\lambda_R (1 - \cos x \cos y)\) | \(d_{23}\)  | \(-\lambda_R \cos x \sin y\) |
| \(d_4\)     | \(-\sqrt{3}\lambda_R \sin x \sin y\) | \(d_{24}\)  | \(\sqrt{3}\lambda_R \cos x \cos y\) |

Table 1. Expressions of coefficients in (14) from Ref[8]

When \(\lambda_R = 0, \lambda_v = 3\sqrt{3}\lambda_{SO}\), the system is an insulator. When \(\lambda_R = 0, \lambda_v < 3\sqrt{3}\lambda_{SO}\), the system is a QSH system where the state can be considered as superposition of two independent quantum Hall
states with different spin orientations. The paired states that connect the valence bands and the conduction bands are called edge states. Here, although the total Chern number $n = n_+ + n_-$ becomes zero, yet their difference $n_+ - n_- = \pm 2$ characterizes the special system. However, when $\lambda_\parallel \neq 0$, spin of electrons cannot be separately treated any more, so Kane and Mele introduced $Z_2$ index from the Bloch wave function. Briefly, the $Z_2$ index can be obtained by counting the number of pairs of complex zeros of $P$, where $P$ is defined as

$$
P(k) = Pf\left[ \begin{pmatrix} u_i(k) & |\Theta| u_j(k) \end{pmatrix} \right]
$$

(15)

$Pf$ represents the Pfaffian of the matrix, $\Theta$ is the time reversal operator and $u(k)$ is the band wave function.

The diagram of energy bands for a 1-dimensional stripe with zigzag boundary condition of both QSH phases and insulating phase is shown in Figure 3.

![Figure 3](image3.png)

Figure 4. (a) QSH phases with $\lambda_\parallel = 0.1t, \lambda_{SO} = 0.06t, \lambda_g = 0.05t$. (b) Insulating phase with $\lambda_\parallel = 0.4t, \lambda_{SO} = 0.06t, \lambda_g = 0.05t$.

After Kane and Mele model was proposed, Fu and Kane[9] introduced an approach to determine the $Z_2$ invariant. The $Z_2$ invariant for 2D situation is given by

$$
(-1)^y = \prod_{i=1}^4 \frac{\text{det}(w(\Gamma_i))}{Pf(w(\Gamma_i))}
$$

(16)

where $w(\Gamma_i)$ is a unitary matrix whose components are defined as $w_{mn}(k) = \langle u_m(-k) | \Theta | u_n(k) \rangle$. $\Theta$ is the time-reversal operator satisfying $\Theta^2 = -1$. Methods of calculation for 3D cases and systems with inversion symmetry were also introduced in Fu and Kane’s work in 2006[9] and 2007[10].

3.3 HgTe/CdTe quantum wells
The model of mercury telluride-cadmium telluride quantum wells exhibiting the topological property, QSHE, was proposed by Bernevig et.al.[11] in 2006. The transition between topologically trivial state and topologically nontrivial states of the sandwich-like heterostructure of HgTe/CdTe is determined by the critical thickness $d_c$ ($\approx 6.3nm$) of quantum wells. A schematic of the structure of the quantum well is shown in Figure 5.

![Figure 5](image5.png)

Figure 5. The sandwich-like structure of HgTe/CdTe quantum wells

In the quantum wells system, an odd number of pairs of helical edge states which are stable and robust against many-body interaction or scattering is protected by the time reversal symmetry where we can write the relationship of two edge states as $\langle -k, \downarrow | \Theta | k, \uparrow \rangle = \hat{T} \langle k, \uparrow | k, \uparrow \rangle$. What really helps the realization of the QSH state is actually the unique inverted band gap of HgTe. As seen in Figure 6,
CdTe has a normal band pattern where s-type $\Gamma_6$ band lies above the p-type $\Gamma_8$ band, while HgTe goes just the opposite, so even before the theoretical model was explored, one could get a glimpse of the potential of such a combination.

![Figure 6. Bulk energy spectrum near the center of BZ](image)

In the deduction of the effective Hamiltonian, Bernevig, Hughes and Zhang took two subbands, E1 and H1, into account and block-diagonalized the Hamiltonian as

$$H_{\text{eff}}(k_x,k_y) = \begin{pmatrix} H(k) & 0 \\ 0 & H^*(-k) \end{pmatrix},$$

$$H(k) = \epsilon(k) + d_i(k)\sigma_i \quad (i=1,2,3)$$

where $\sigma_i$ are Pauli matrices. Among parameters above, $d_i(k)$ contains a consequential mass parameter $M$ which would change its sign leading to band inversion with the thickness of the HgTe layer varying. The existence of helical edge states can be revealed more explicitly by solving the eigenvalue problem of the effective Hamiltonian, although the form of the effective Hamiltonian and the sign reversal phenomenon have shed light on QSHE.

### 3.4 Other 2DTIs predicted theoretically

Beyond the models introduced previously, lots of two-dimensional topological insulators have been predicted theoretically in the recent ten years. In 2011, ultrathin Bi(111) films with nontrivial $Z_2$ index was found theoretically where the topology property of it is independent of the thickness of the material[12]. Besides, atomically thin crystals[13] like silicene, germanene and stanene which possess a stronger SOC than graphene are predicted to be 2DTIs according to first principle calculation[14, 15]. SnX[16], PbX[17], BiX/SbX[18] ($X=\text{H, I, Br, Cl, F or OH}$ for SnX, $X=\text{H, I, F, Cl, Br}$ for PbX and $X=\text{H, F, Cl, Br}$ for BiX/SbX) were also predicted to be 2DTIs, among which BiX/SbX have large band gaps ranging from 0.74 to 1.08eV and are also promising for room temperature application. Another QSH insulator, GaBiCl$_2$, with strong SOC and large energy gap is also predicted to be hopeful candidate for achieving dissipationless transport devices in 2015[19]. Further addition to the family of 2DTIs consists of silicon based chalcogenide[20], functionalized Thallium Antimony films[21], etc. In 2016, VA-VA semiconductors, like $\beta$-SbAs, were explored and were considered to be candidates for QSH systems[22]. Among the large family of 2DTIs predicted theoretically, transition metal dichalcogenides (TMD) may be one of the most promising candidates for achieving room temperature QSHE. Since its prediction in 2014[23], extensive work has focused on this family and its structurally distorted phase[24-32]. Notably, these study of QSHE in 2D topological insulators has built up a broad platform for engineering topological insulators by means of strain, tension, electrical and magnetic regulation, optical probe, proximity effect and so on and survival of QSHE has been proved above liquid nitrogen temperatures, which aggrandizes the application value of 2D TIs.
4. Conclusion

To sum up, topological insulators came into public attention through reheating Haldane’s work[2] in 1988, which inspired people to consider possibility of topologically nontrivial properties among numerous materials with zero external magnetic flux. Subsequently theoretical and calculative work on searching for topology in seemingly trivial places based on topological band theory sprang up. It turns out that topology hiding in edges and surfaces prepares plentiful surprises for us. Based on the creative work of topological insulators, there emerge a large number of topologically nontrivial condensed matter materials like topological superconductors[33, 34], topological crystalline insulators[35-40], topological Kondo insulators[41], topological Mott insulators[42], some complex oxides[43, 44], Weyl semimetals, etc. The development in this area has greatly enhanced our understanding of different phases like magnetism, superconductivity, and spin of topological materials. However, topological insulator is a discipline in babyhood and still has a long way to go before widespread pragmatic application. In order to get deeper understanding of TIs and other related realms, more profound mathematical tools in topology beyond band theory need implementing and probing. Nevertheless, it is beyond doubt that further probe into the family of topological materials will lead to significant progress in superconductivity, spintronics and quantum computation.

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