The identifying features of topological insulators

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This paper presents the basis through which we define topological insulators. First, we provide a brief overview of the justification and history of classifying material phases as topological, followed by a streamlined examination of what defines a topologically insulating phase, with a focus on 2D systems. Herein, we discuss that a topological insulator has strong spin-orbit coupling and preserves time reversal symmetry. The combination of these traits results in conductive edge states that are protected by their band structure topology and ordered by spin. This makes topological insulators an attractive material for the development of spintronic devices. Finally, we present the first experimental evidence of a 2D topological insulator.

INTRODUCTION

Since topological insulators (TIs) were theoretically predicted in 2005, there has been a growing effort to discover and understand materials with a TI phase.[1][2]

TIs present a potential avenue to spintronics, the field of designing electronics based on the control of spin degrees of freedom.[3] Making use of spin degrees of freedom in electronic data storage allows for more information to be stored per electron, theoretically resulting in a significant reduction in power consumption relative to traditional electronics. The field of spintronics is still predominantly in its conceptual phase, so the ways in which TI materials would be utilized in these applications are still in development.[4]

When the TI phase was first introduced, it was suggested that graphene may display it.[1][2] However, this has yet to be experimentally confirmed due to challenges in maintaining strong spin-orbit coupling at experimental temperatures.[5] Subsequently, it was suggested that the TI phase could be observed in CdTe/HgTe/CdTe quantum wells, which was indeed experimentally confirmed.[6][7] Since that first confirmation, the TI state has been observed in $Bi_{1-x}Sb_x$, Sb, Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3, using ARPES, STM, and STS measurements.[5][8]

As a result of this growing search for new materials with a TI phase, examining materials and suggesting they may have a TI phase has become a trend in experimental condensed matter research.[5][9] However, without proceeding with a firm grasp of what defines a TI phase, these claims could go unchecked. This paper hopes to act as a brief review of what defines a TI phase, to assist the reader in understanding those claims.

CLASSIFICATION OF STATES BY TOPOLOGY

Historically, the phase of a material has been defined using Landau theory, which requires the breaking of an underlying symmetry for a process to constitute a phase change. However, a new phase classification method was introduced during the 80's and 90's.[10][11] It was suggested that phases could also be defined by their 'topological order'. The topological order of band structures is analogous to the topology of a 2D surface, which is traditionally classified by its genus. Similar to symmetry in Landau theory, the topological order is a fundamental property of a material's band structure that remains constant under continuous changes in the Hamiltonian. The measurable invariant property of the material can be different for different topological orders. Then, if the specified fundamental property of a topological phase was observed to change, it must be accompanied by a topological phase change.[9]

When we consider the electronic properties of a material, one might imagine labelling any material state, ranging from a semiconductor with a Dirac point, to the vacuum as an insulator. However this sort of classification, based on a finite band gap, is not necessarily productive - not all materials classified as an insulator by this definition are topologically equivalent.[12] Herein lies another benefit of the topological classification system: it explains unexpected electronic behaviour from band structures that otherwise look similar.

The Integer Quantum Hall Phase

The idea of classifying material phases by their topological order was motivated by the introduction of the integer quantum Hall (QH) phase.[12] While the integer QH phase is not equivalent to a TI phase, the TI phase is often described in relation to the QH phase, which makes it a logical starting point for this discussion.

When electrons bound in two dimensions are placed in a strong external magnetic field, the electrons will orbit in a circular pattern with a cyclotron frequency, ω_C, as is illustrated in Fig.1. The system is then analogous to a harmonic oscillator with energy levels dependent on the cyclotron frequency, called Landau levels.[13] The levels are degenerate for a large range of allowed momenta, made finite only by the physical bounds of the material.

The resulting electronic behaviour of the material is then related to the filling fraction of the highest occupied Landau level.

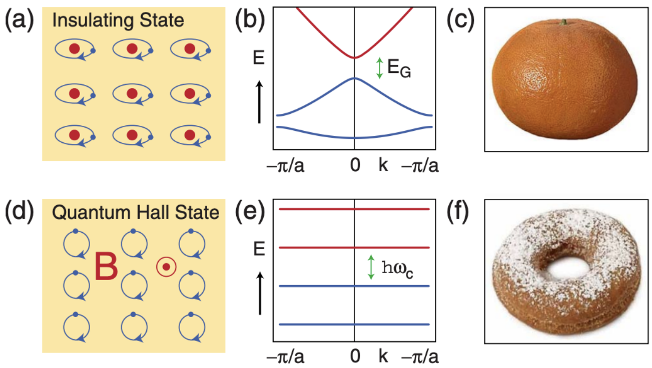

FIG. 1: Illustration of the difference between a common insulator and a QH insulator. (a) Diagram of electron behaviour in a common insulator. (b) Band structure of a common insulator. (c) Example of a geometric shape with the genus = 0. (d) Diagram of electron behaviour in a QH state. (e) Landau level structure for a QH state. (f) Example of a geometric shape with the genus = 1 as a result of its hole. Figure taken from [9].

As with the classical Hall effect, a Hall voltage results from this current of orbiting electrons, creating a uniform electric field. For a system with periodic boundaries, this would lift the degeneracy of the Landau levels. However, without periodic boundaries, the behaviour at the edges of the material must be treated carefully. As one might predict from the classical Lorentz force, this electric field generates a one-way current along the edge of the material. The unilateral direction of this current is referred to as a 'chiral' state. We can then measure the conductivity of this chiral state, which can be described by equation (1).

$$\sigma_{xy} = \frac{n \cdot e^2}{2\pi\hbar} \tag{1}$$

where n is the number of filled Landau levels.[9] The significant finding here is the quantized nature of σ_{xy}, something that would not be found in a normal insulator. In fact, the quantum nature of the QH state's conductivity was found to be exceptionally robust to smooth changes in the electron density.[14] The explanation for this stable quantum nature of the Hall conductivity was provided by Thouless, Kohmoto, Nightingale, and den Nijs.[10] They stated that the integer n in equation (1), referred to as a 'Chern invariant', is defined by the topology of the band structure. Specifically, we are interested in how the edge states' bands connect the bulk valence and bulk conduction bands. Further discussion on what is meant here by topology will be continued in our discussion of the TI phase.. Because it is determined by topology, the Chern invariant is analogous to the genus of a 2D surface in mathematics.[15] This invariant parameter of the QH state is what defines a topological state as different from a normal insulator under the same external conditions.

Another way the Chern invariant can be understood is by the Berry phase.[16] Generally, the Berry phase is a phase factor applied to eigenstates when they experience a cyclical variation in the Hamiltonian. For example, if we take a closed line integral of an eigenstate in reciprocal space, the eigenstate would obtain a Berry phase. From the Berry phase we can define the Berry flux, which is analogous to magnetic flux.[17] Then, if you take a surface integral over the Brillouin zone of the Berry flux, you get the Chern number of a Landau level as shown in equation (2).

$$n_L = \frac{1}{2\pi} \oint_{BZ} d\boldsymbol{S} \cdot \boldsymbol{F}_L(\boldsymbol{k}) \tag{2}$$

Where $\boldsymbol{F}_L(\boldsymbol{k})$ is the Berry flux. Note here that n_L is only the Chern number for an individual Landau level - generally when the Chern invariant is discussed, we are considering the sum of Chern numbers from all occupied Landau levels.

At the interface of two different topological states, such as the edge of a topological material and a vacuum, the band gap must go to zero so that the topological variant can change across the boundary. This forced conductive state is precisely the same as the one-way current induced by the QH effect mentioned earlier.

Now that we have discussed the integer QH state, we will examine the TI phase and what makes it unique topologically.

THE TOPOLOGICAL INSULATOR PHASE

Unusually, the TI phase was described theoretically before being observed experimentally. Its existence was predicted based off the concept of the quantized conductance of the QH state.[1][2] In fact, one can think of a 2D TI state as the superposition of two QH states with opposing Hall conductance values, leading to a net vanishing Hall conductance. As a result of the similarities, the 2D TI phase is also often referred to as the quantum spin Hall phase (QSH). For the following discussion, we will examine only the TI phase in 2D for brevity, however it may be scaled up to 3D, where it exhibits additional properties.

The TI phase shares many similarities to a QH phase, with the exception that it need not be under the influence of an external magnetic field. Instead, a TI phase arises from strong spin-orbit coupling, also called Rashba coupling.[18] This results in spin-momentum locking, where the magnetic field generated from the momentum of the electron's cyclical orbit 'locks' the electron's spin axis. Spin-orbit coupling is itself a relativistic effect, relying on the interaction of a particle's spin with the apparent magnetic field seen from an electron's reference frame. The consequence of this locking is the generation of spin currents along the edge of the material, as drawn in Fig. (2). Again, this can be tangibly thought of as two opposing QH edge states, referred to as a singular 'helical state'. These edge spin currents are what make TI materials potentially useful in spintronics, which aims to control spin degrees of freedom.

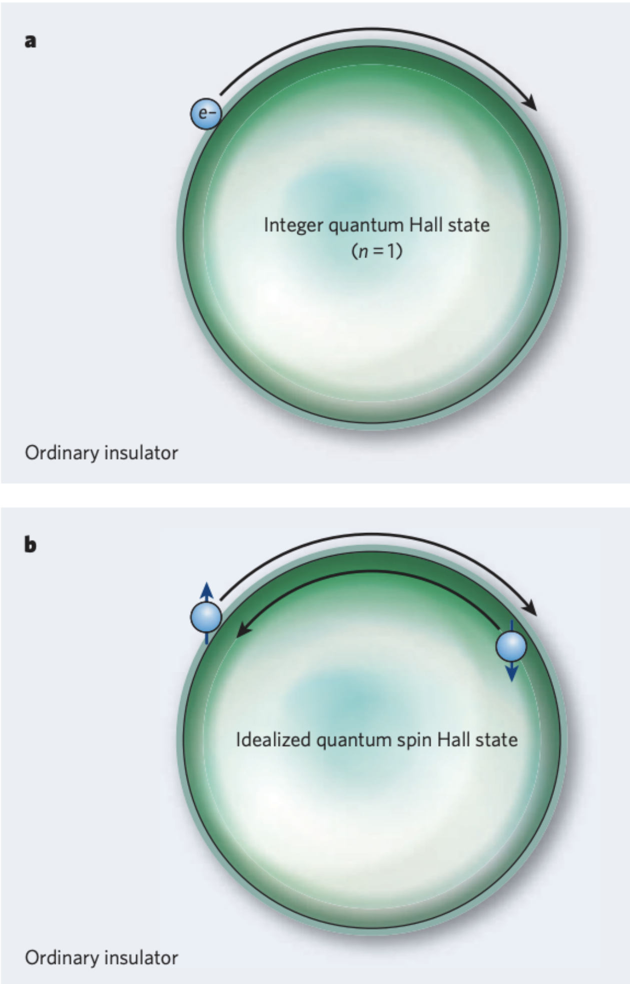

FIG. 2: Diagram of the intrinsic edge states of QH phase and TI phase. (a) 2D QH phase surrounded by a common insulator with a drawing of the chiral conductive edge state. (b) 2D TI phase surrounded by a common insulator. Drawing of paired conductive edge states with locked spins, analogous to a superposition of two QH states. This pair of conductive edge states is also referred to as 'helical state'. Figure taken from [19].

Most notably, since the TI phase isn't under an external magnetic field, time-reversal symmetry (TRS) is maintained. In other words, the TI state is even in TRS, while the QH state is odd. The implications of preserving TRS will help to explain the differences between QH and TI phases. First, keeping TRS means that the band structure must be symmetric about $\vec{k} = 0$. Another thing we quickly notice is that the Hall conductance is odd under TRS, so although it was a convenient quantized measurable property of a QH phase, it vanishes in a TI phase.[9]

TRS symmetry is an antiunitary operator as per equation (3):

$$\hat{T} = K \cdot exp\left(\frac{i\pi\hat{S}_y}{\hbar}\right) \tag{3}$$

where $\hat{S}_y$ is the spin operator along the y-axis, and K denotes complex conjugation. Its antiunitary property means that $\hat{T}^2 = -1$. As a result, in order for a state to be an eigenstate of $\hat{T}$, it must be at least doubly degenerate. This assertion is called Kramers theorem.[20] For a system without spin-orbit coupling, Kramers theorem trivially amounts to enforcing the degeneracy of spin up and spin down electrons. However, spin-orbit coupling lifts this degeneracy. Consequently, in order for Kramers theorem to hold in a system with spin-orbit coupling, we must enforce double degeneracy at the points where momentum preserves TRS. These 'Kramers degenerate' points in the Brillouin zone are $\vec{k} = 0, \pm\frac{\pi}{a}$. Outside of these special points, the spin-orbit coupling lifts the degeneracy of the states with opposing spins, as expected. This is shown diagrammatically in Fig. 3.

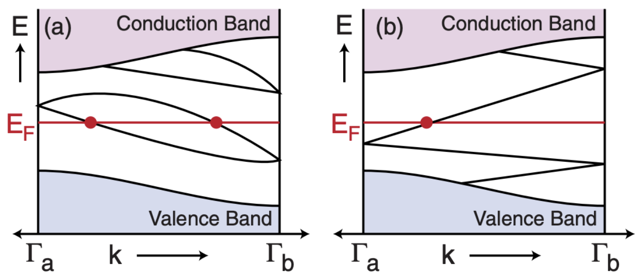

FIG. 3: Band structure over half of the Brillouin zone of an insulating material with conductive edge states. Here, the black lines between the valence and conduction bands show the conductive edge states. The points Γ_a, Γ_b are the Kramers degenerate points at momenta 0 and $\frac{\pi}{a}$ respectively. In panel (a), there are an even number of intersections with the Fermi energy, E_F. In panel (b), there are an odd number of intersections with E_F, and thus the conductive states are topologically protected. Figure taken from [9].

The important feature to examine in the band structure is thus the number of boundary states that cross the Fermi energy, E_F. If an even number of states cross E_F, then one could imagine smoothly changing the Hamiltonian in order to have a E_F that is crossed by no edge states. However, if an odd number of states cross E_F, then no matter what smooth changes are made to the Hamiltonian, there will always be at least one state crossing E_F. Herein lies arguably the most significant feature of a TI state - it has an odd number of crossings of E_F, and so nothing short of altering the topology of the band structure can eliminate its conductive edge states.

This feature is characterized using the '$\mathbb{Z}_2$ invariant', ν, as opposed to the Chern invariant used for the QH phase. Equation (4) is a way to express the change in ν across an interface:

$$\Delta\nu \bmod 2 = N_K \tag{4}$$

where N_K is the number of Kramer degenerate states that cross E_F.[21] Following from our preceding discussion, a material with $\nu = 1$ is a TI state, while $\nu = 0$ denotes a topologically trivial state.[22] In addition to equation (4), there are numerous additional ways to define the $\mathbb{Z}_2$ invariant that utilize tools from the mathematics of topology.

At this point, the reader may be wondering: if the Hall conductance used for the QH phase is vanishing in the TI phase, by what measurable value can we detect a TI phase? The simplest measurement that shows a 2D TI state is by measuring its 'longitudinal conductance', G. We will not derive it here for brevity, but we use the result that every quantum channel has $G = \frac{e^2}{2\pi\hbar}$.[23] A 2D TI state has one helical state on either edge, leading to the theoretical longitudinal conductance of $G = 2 \cdot \frac{e^2}{2\pi\hbar}$. The first 2D TI phase to be experimentally measured was in CdTe/HgTe/CdTe quantum wells. As shown in Fig. (4), König *et al.* measured G of the quantum wells in their TI state to match this theoretical value.[7]

In summary, a topological insulator is a material that exhibits a TI phase. The TI phase is a result of strong spin-orbit coupling and time reversal symmetry. It is characterized by a $\mathbb{Z}_2$ invariant which relates to the topology of its edge state band structure. As a result, the spin-conductive nature of its edge states is protected under smooth modulations to the Hamiltonian. These protected intrinsic spin currents make the TI state ideal for the development of exotic spintronic devices.

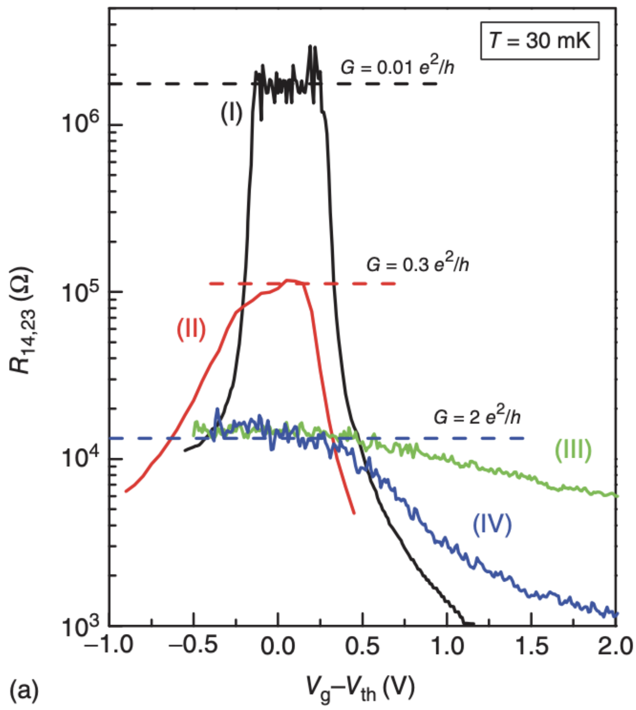

FIG. 4: Transport measurement of CdTe/HgTe/CdTe quantum wells of varying thickness. Samples (III) and (IV) have thicknesses past the critical topological phase transition value and are found to have the theoretical longitudinal conductivity of $G = 2 \cdot \frac{e^2}{2\pi\hbar}$. This figure demonstrates the first experimental evidence of a TI phase. Figure taken from [5].

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