Quantum spin Hall systems and topological insulators

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Abstract. Topological insulators (quantum spin Hall systems) are insulating in the bulk but have gapless edge/surface states, which remain gapless even when nonmagnetic disorder or interaction is present. This robustness stems from the topological nature characterized by the $Z_2$ topological number, and this offers us various kinds of new novel properties. We review prominent advances in theories and in experiments on topological insulators since their theoretical proposal in 2005.

Topological insulators are insulating in the bulk but have gapless edge/surface states, which carry a pure spin current. They are also called quantum spin Hall systems, because they are the ‘gapped’ analogues of spin Hall systems, just as the quantum Hall effect is to the Hall effect. The gapless states are protected topologically as long as the time-reversal symmetry is preserved. Since they were first proposed in 2005 [1–3], there have been a number of interesting theoretical proposals as well as experimental observations on their novel properties. Unlike the edge/surface states of ordinary insulators, which depend crucially on the edge/surface conditions, the existence of edge/surface states in topological insulators does not depend on the edge/surface conditions, but comes from bulk properties.

Two-dimensional (2D) topological insulators are characterized by the $Z_2$ topological number $\nu = 0, 1$, which corresponds to ordinary and topological insulators, respectively. The $Z_2$ topological number $\nu$ is defined from the bulk Bloch wavefunctions, and therefore the topological insulator is a bulk property. There are several equivalent ways of defining the $Z_2$ topological number [2, 4, 5], from which various novel properties are derived. On the other hand, in 3D topological insulators [6–8], there are four $Z_2$ topological numbers, $\nu_0 : (\nu_1, \nu_2, \nu_3)$, where
$v_i = 0, 1$ [9]. Among these four numbers, $v_0$ is the most important because the number $v_0$ gives the distinction between a strong topological insulator (STI) ($v_0 = 1$) and a weak topological insulator (WTI) ($v_0 = 0$). If $v_0 = 1$ the system is an STI, where gapless surface states exist on every surface, irrespective of the details of the surface. On the other hand, when $v_0 = 0$, the system is a WTI, where gapless states may be absent on some surfaces. Other topological numbers $v_1$, $v_2$ and $v_3$ give information on dispersions and topology of the Fermi surfaces of surface states. Because these phases with a bulk gap are characterized by the $Z_2$ topological numbers, they can change only when the bulk gap closes by changing some parameter in the system [10, 11]. For the STI, one typical dispersion for the surface states is the Dirac cone, i.e. the cone-shaped dispersion, similar to graphene.

In real materials the wavefunctions are not necessarily of the Bloch form, whereas the distinction between the topological and ordinary insulators remains. The edge states of the 2D topological insulator have a novel property that elastic backscattering by nonmagnetic impurities is prohibited [12, 13]. Therefore, the edge states remain gapless, and the topological insulator phase is not destroyed [14–16]. Associated critical phenomena have been studied numerically [17–19]. Magnetic impurities, on the other hand, open a gap to the edge states. The physics of the topological insulator survives also in the presence of interaction, as has been discussed theoretically [12, 13, 20–22].

For candidate materials for 2D topological insulators, the first proposal is bismuth (Bi) ultrathin film [23], because of the strong spin–orbit coupling in Bi. The HgTe quantum well is then proposed to be a topological insulator [24]. In this quantum well, the HgTe layer is sandwiched between CdTe, and if the thickness of the HgTe layer is higher than the critical thickness $d_c \sim 6.5$ nm, it becomes a 2D topological insulator because of the inverted band structure of the semiconductor HgTe. This theoretical proposal has been verified experimentally [25–27]. The edge states form perfectly conducting channels, and transport measurement shows novel properties, such as quantized conductance $2e^2/h$ [25] and nonlocal quantized conductance [27].

For 3D topological insulators, when the time-reversal symmetry is broken by an external magnetic field or by growing a magnetic film on the surface of the topological insulator, a gap opens for the otherwise gapless surface states. The surface states then become quantum Hall states with $\sigma_{xy} = \pm e^2/4\pi$. This gapped surface state with $\sigma_{xy} = \pm e^2/4\pi$ shows the magneto-electric effect [28–30]. When a 3D topological insulator is attached to a superconductor, the surface states will become gapped via the proximity effect. Dirac cones are special in that around the attached superconductor there appear Majorana fermions, which are promising tools for quantum computation [31, 32].

So far there are various proposals for materials and experimental measurements. Here we introduce a few of them. Bi$_{1-x}$Sb$_x$ is theoretically proposed to be a 3D topological insulator [9]. Bi and Sb are both semimetals, while Bi$_{1-x}$Sb$_x$ with $0.07 < x < 0.22$ becomes a topological insulator. The surface states of this material with $x \sim 0.10$ are measured by angle-resolved photoemission spectroscopy (ARPES) [33]. It is observed that there are five Fermi surfaces of the surface states between $\Gamma$ and $M$ points, showing that Bi$_{1-x}$Sb$_x$ is the STI. For stronger evidence of the topological insulator, the spin states of the surface states should be determined. It has been done with spin-resolved ARPES [34, 35], showing that the individual Fermi surfaces are not spin-degenerate, and have specific spin states. Instead of the complicated Fermi surfaces of the surface states in Bi$_{1-x}$Sb$_x$, other materials with simpler Fermi surfaces have been pursued. It is then theoretically proposed [36] that Bi$_2$Te$_3$, Bi$_2$Te$_5$ and Sb$_2$Te$_3$ are topological insulators.
The surface states of $\text{Bi}_2\text{Te}_3$ and $\text{Bi}_2\text{Se}_3$ have been measured by ARPES [37, 38], revealing that the dispersion of the surface states is a single Dirac cone around the $\bar{\Gamma}$ point. The spin-resolved ARPES shows that these states are not degenerate and have a fixed spin direction, clockwise in the wavenumber space if the Fermi energy is above the Dirac point [39]. Unlike graphene, there is only one Dirac cone in the Brillouin zone, and consequently, the surface states are proposed to show no Anderson localization [40].

In this Focus Issue of *New Journal of Physics* [41–54], we look at various aspects of novel physics of topological insulators. One of the fundamental issues is the $Z_2$ topological number. The $Z_2$ topological number has various expressions obtained from different viewpoints, such as the expression with Pfaffian in Hamiltonian formalism [4] and that from the field-theoretical method [28]. As their starting points are different, it is not straightforward to relate them to each other. In [41], their equivalence is shown directly for the first time. In [42], the topological number is understood as an obstacle to define the wavefunctions smoothly in the Brillouin zone with some constraint related to time-reversal symmetry. Thereby the four $Z_2$ topological numbers in 3D can be understood from the $Z_2$ topological numbers in 2D. This gives an intuitive understanding of the four $Z_2$ topological numbers in 3D. In [43], a related subject of the gauge field structure for a time-reversal symmetric system is discussed. Many-body systems with Kramers degeneracy are formulated by using quarternions, and the gauge field and topological numbers are discussed with the language of quarternions. This reveals the close relationship between the $Z_2$ quantization and the Kramers degeneracy.

The development of topological insulators has brought about new fields in field theory. In [44], critical properties of topological insulators have been discussed using the SU(2) network model. The authors construct the SU(2) network model, and derive the Dirac Hamiltonian from the network model. From its clean limit, the authors show that the $Z_2$ topological number corresponds to the SU(2) Wilson loop. The authors also study this network model numerically and discuss multifractality of the edge states and its connection to the Hamiltonian.

The emergence of the topological insulator has aroused interest in the idea that there might be other new topological classes of Hamiltonian with the gap. Ryu *et al*’s work [45] is like an encyclopedia for the classification of topological phases. The paper classifies topological insulators and superconductors in each spatial dimension and in various symmetries. By using dimensional reduction, the authors construct the field theory for various topological phases from other topological phases in higher dimensions. They make an exhaustive list of topological insulators and superconductors, and find that there is an eightfold periodicity in dimensions. The argument here is strong and general, because it only relies upon symmetry and dimensions and not upon details of the systems.

Topological numbers characterizing the topological insulators have been formulated in a mathematically rigorous way in [46]. The paper reviews analytic tools for topological insulators, with the aid of noncommutative calculus and geometry. It shows how to put physical arguments developed in the field of topological insulators into a rigorous framework in mathematics.

For 2D topological insulators, motivated by the first theoretical work [24] in the HgTe quantum well, various transport experiments have been reported, and the theory so far is based on the four-band model constructed. In [49], the authors include inversion symmetry breaking and the in-plane potential, and derive the four-band model by the $k \cdot p$ perturbation theory. As a result, in addition to the four-band model in [24], the Rashba term and in-plane Pauli term appear. The authors use a tight-binding model constructed from this model to calculate the spin Hall conductance.
Experimental observations of the topological insulators are reported. For 3D topological insulators, the surface states are measured in [47] and [48] by ARPES. In [47], Sb and Sb$_{0.5}$Bi$_{0.1}$ are studied by ARPES, and the results are compared with the first-principle calculations. Although Sb itself is a semimetal, the topological classification is possible because the direct gap is nonzero everywhere in the Brillouin zone. In agreement with the theory, Sb is shown to be topologically nontrivial, and has surface states traversing across the direct gap. The measurement in [47] also shows that Sb$_{0.5}$Bi$_{0.1}$ is similar to Sb. In [48], the surface states of Bi$_{1-x}$Sb$_x$ ($x = 0.04$, 0.12–0.13) are studied by ARPES. The previous theories suggest that Bi$_{1-x}$Sb$_x$ with $x = 0.04$ is an ordinary insulator and Bi$_{1-x}$Sb$_x$ with $x = 0.12$–0.13 is a topological insulator. By comparing the ARPES data for the two cases, the above expectations are clearly verified. Moreover, for the topological insulator ($x = 0.12$–0.13), the authors identify the mirror chirality out of their ARPES data.

The effect of disorder in 3D topological insulators is studied in [52]. By using the effective model of the Dirac Hamiltonian, disorder of various types is studied within the self-consistent Born approximation. As a result, the phase diagram and the quantum correction to conductivity are obtained from microscopic calculations.

First-principle calculations are powerful for the investigation of the physics of topological insulators. In [50, 51, 53, 54], calculations for various candidates of topological insulators are presented. In [51], the 3D topological insulators Bi$_2$Te$_3$, Bi$_2$Se$_3$ and Sb$_2$Te$_3$ are studied by first-principle calculations. They show the profiles of the surface states and their penetration depths. The spin-resolved Fermi surface is also demonstrated. Because Sb$_2$Se$_3$ is an ordinary insulator, a phase transition between the topological and simple insulators is expected in Sb$_{1-x}$Se$_x$ when $x$ is varied. The first-principle calculation verifies that it indeed occurs at about $x = 0.94$. In [50], a systematic study of the films of Bi–Sb alloys is conducted, motivated by the theoretical and experimental study of Bi–Sb alloys [9, 34, 35] as topological insulators. Various structures have been studied, including ordered alloy with layers of –Bi–Sb–Bi–Sb– and –Bi–Bi–Sb–Sb–, and (111) ultrathin films with similar arrangements. The bands close to the $\Gamma$ point differ across various types of alloys. On the other hand, the Bi–Sb film in the (110) orientation is shown to be gapped due to the buckling. In [53], the ternary tetradymite-like compounds $M_2X_2Y$ ($M = \text{Bi, Sb}$; $X = \text{S, Se, Te}$) are studied by first-principle calculations. Bi$_2$Se$_2$S, Sb$_2$Te$_2$Se, Sb$_2$Te$_2$S, Bi$_2$Te$_2$Se and Bi$_2$Te$_2$S are found to be topological insulators. In particular, the first three have surface states consisting of an isolated Dirac cone. In [54], quaternary chalcogenide (I$_2$–II–IV–VI$_4$) and ternary famatinite (I$_3$–V–VI$_4$) compounds are examined by first-principle calculations. The authors of [54] study Cu-based compounds and find a number of topological insulators such as Cu$_3$SbS$_4$ and Cu$_2$ZnGeSe$_4$. Topological phase transition is studied for tuning between Cu$_2$ZnSnS$_4$ (trivial insulator) and Cu$_3$SbS$_4$ (topological insulator). The tuning is simulated by a change of the atomic numbers of constituent elements, and band inversion at the $\Gamma$ point is found.

To summarize, papers [41–54] of the Focus Issue present significant results on various aspects of topological insulators and would be of importance for further progress in the field.

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