Daniel McCulley
May 6, 2016
Summary of the field

Topological Insulators

Introduction

Since the dawn of the field, a primary focus of condensed matter physics has been the discovery of new states of matter. Most phases of matter are connected to some form of symmetry in the system, and phase changes are often associated with breaking that symmetry. A brief description of the connection between phases of matter and symmetry is that because physical laws are invariant under different symmetries, if the symmetry changes drastically then the behavior of the system will as well. One common examples are magnets, whose order is associated with breaking rotational symmetry. A less straightforward example is superconductors, whose order is associated with breaking gauge symmetry.

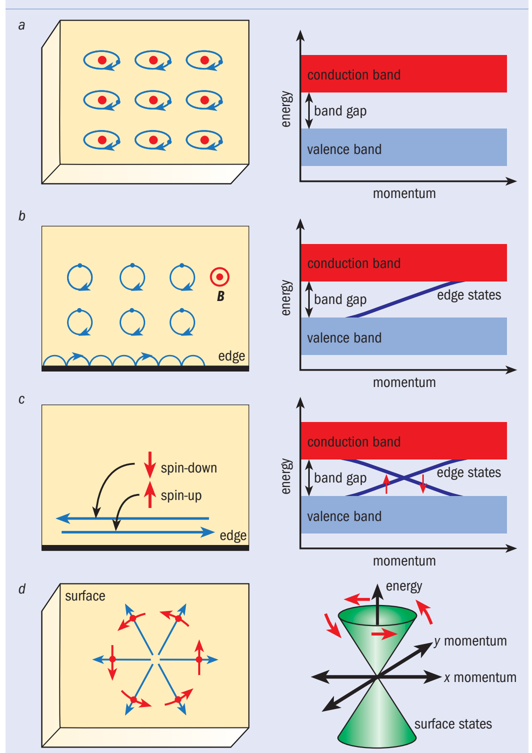
Topological Insulators (TIs), and topologically protected states in general, are a state of matter of particular interest because they deviate from the general description of phases and symmetries above. The phase does not emerge through breaking of a symmetry in the system, but rather through particular quantum states that happen to exhibit time reversal (TR) symmetry. It's worth noting that in general, many systems (including a normal insulator) do not possess TR symmetry, and the universe as a whole does not. Thus, the symmetry-breaking associated with a transition from a topological insulator to a normal insulator is TR symmetry.

Topological insulators are characterized by having robust, highly conductive states on the surface or edge of an otherwise insulating material. The states are robust in the sense that they topologically protected from by scattering sources, and are sometimes referred to as dissipation-less conducting states. This phenomenon presents a long sought after solution to power dissipation in integrated circuits, one of the main obstacles in shrinking the technology. Others are interested in their use in spintronics and error tolerant quantum computation. Recently, further interest has been expressed in using TIs to detect majorana fermions at the interface with a superconductor [12].

Materials with highly conductive surface states that are not protected from scattering are not considered topological insulators. A topological state is one that is protected under any continuous transformation in the system. A continuous transformation in the context of of an insulator is any change in the Hamiltonian of the system that doesn't eliminate the band gap. There are two conditions required for topologically insulating states to form, which is that the state exhibits TR symmetry and that there is a strong spin orbit coupling (SOC) between electrons spin and their orbital momentum. The importance of SOC and TR symmetry is discussed further in the next section.

The first discovery of a topologically protected state was the quantum hall (QH) state (von Klitzing et al., 1980). Physicists at the time were surprised to see that in the presence of large magnetic fields, the Hall conductance is quantized at integer values of e^2/h independent of sample quality and size. The term *topological invariant* has become a useful concept. It describes a quantity like the Hall conductance; one which is invariant under small changes in the material. Topological invariants take the form of an integral whose integrand may vary locally, but whose value is invariant and instead depends only on the most general properties of the system.

1 Electronic states of matter



(*a*) The insulating state is characterized by an energy gap separating the occupied and empty electronic states, which is a consequence of the quantization of the energy of atomic orbitals. (*b*) In the quantum Hall effect, the circular motion of electrons in a magnetic field, ***B***, is interrupted by the sample boundary. At the edge, electrons execute "skipping orbits" as shown, ultimately leading to perfect conduction in one direction along the edge. (*c*) The edge of the "quantum spin Hall effect state" or 2D topological insulator contains left-moving and right-moving modes that have opposite spin and are related by time-reversal symmetry. This edge can also be viewed as half of a quantum wire, which would have spin-up and spin-down electrons propagating in both directions. (*d*) The surface of a 3D topological insulator supports electronic motion in any direction along the surface, but the direction of the electron's motion uniquely determines its spin direction and vice versa. The 2D energy–momentum relation has a "Dirac cone" structure similar to that in graphene.

2D Topological Insulators

Theory

The 2D topological insulator, or quantum spin Hall (QSH) state, can be understood well in comparison with the QH state. The presence of the magnetic field in the QHE causes electrons to move in circular paths, illustrated in Figure 1a (image and caption taken from [7]). On the edge of the material the circular path is interrupted. Gapless edge states, sometimes referred to as "skipping" orbits, form that are conductive (Figure 1b).

Only materials comprised of atoms with large nuclei (such as Hg, Bi, and Sb) are predicted to be topological insulators. Their outer electrons have relativistic momenta, giving them a strong SOC. The interaction between the spin and orbital angular momentum plays a role analogous to that of the external magnetic field in the QH state. Spin down and spin up electrons will have an opposite spin orbit interaction, causing spin up edge state to conduct one way while the spin down edge state conducts the other. This is how the effect has earned the name *quantum spin Hall (QSH)* effect. Depicted in Figure 1c are the two gapless edge states of the QSH effect, which are related through time reversal symmetry, as both velocity and spin are odd under time reversal symmetry.

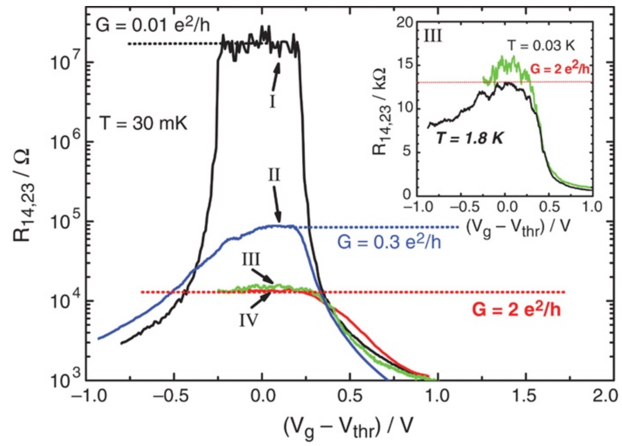


Fig. 2. The longitudinal four-terminal resistance, R14,23, of various normal (d = 5.5 nm) (I) and inverted (d = 7.3 nm) (II, III, and IV) QW structures as a function of the gate voltage measured for B = 0 T at T = 30 mK. Image and caption taken from [3]

Displayed in Figure 1d is an analogy of how this effect generalizes into three dimensions, where surface states move in the direction of their spin. A gapless Dirac cone of surface states is formed connecting the bulk valence and conduction bands. This is discussed further in the 3D topological insulator theory section.

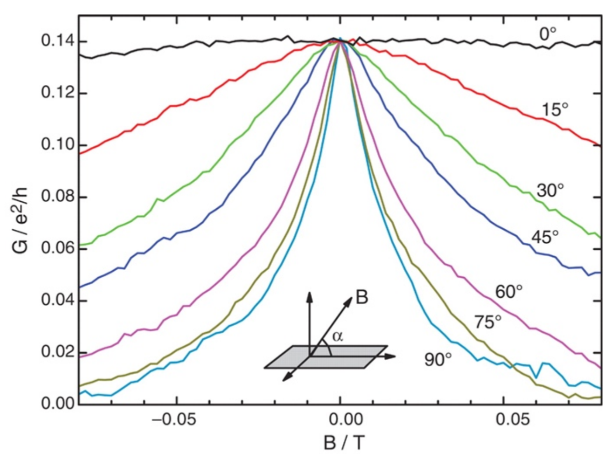


Fig. 3 Four-terminal magnetoconductance, G14,23, in the QSH regime as a function of tilt angle between the plane of the 2DEG and applied magnetic field for a d = 7.3-nm QW structure with dimensions (L × Ω) = (20 × 13.3) μm^2 measured in a vector field cryostat at 1.4 K. Image and caption taken from [3]

Prediction and discovery

In a somewhat unusual fashion for condensed matter physics, the theorists have led the experimentalists in the push for the discovery of topological insulators. The existence of a 2D topologically insulating state was first predicted in 2005 [1] and the first 2D topologically insulating material (HgTe/CdTe quantum wells) was predicted in 2006 [2]. The TI state was subsequently observed in HgTe/CdTe quantum wells in 2007 [3]. The results from the 2007 discovery are displayed in Figures 2 and 3. Figure 2 shows integer quantized values of resistance h/e^2, independent of sample size which alone is strong evidence for a topological insulator. It's also worth noting that the mobility of the electrons reported in this experiment is on the same order as in graphene: $\mu \sim 10^5\ cm^2V^{-1}s^{-1}$, which is considerably higher many bulk material such as silicon where : $\mu \sim 10^3\ cm^2V^{-1}s^{-1}$. Alone, the high mobility doesn't imply that the state is topologically protected. However, in combination with the fact that they see a conductance of G_0 at T=30mK (Fig. 2), the data is very compelling.

Further evidence is seen in the destruction of the TI state though application of a magnetic field which breaks the time reversal symmetry protecting the state. This can be seen in Figure 3, where the conductance goes to zero with increasing magnetic fields perpendicular to the plane of the material.

3D Topological Insulators

Theory

Mathematically generalizing the phenomena of topological insulators to 3D is messy, and the early predictions of such states were complicated. This is why it took an extra 2 years from the prediction of the first 2D TI material to predict the first 3D TI materials. The models have continued to be refined, and simpler special cases have been predicted and observed, but as it stands most of the predicted materials haven't yet been experimentally realized. A qualitative generalization from two to three dimensions can be made fairly easily. A thorough, quantitative explanation of the theory of 3D topological insulators is discussed in [11].

In two dimensions the topological state was characterized by 1D conducting channels on the edge of the material whose propagation direction depended on the spin. This is illustrated in a band diagram (Fig. 1c) as a line connecting the valence and conduction bands. The three dimensional equivalent of the gapless edge states is a surface of states that conduct in the direction of their spin. It is illustrated in a band diagram as a spin polarized cone of topologically protected states connecting the bulk valence and conduction band states, where the spin points tangential to the cone. Both the theoretical and experimental results showing the cone of states are impressive, and are discussed in the next section.

It was sufficient in 2D to measure G_0 near T=0K, independent of sample width, to show evidence of a topological insulator. Experimental detection of the 3D topologically insulating state is more difficult because the conductance isn't expected to be precisely zero at T=0K. The primary technique used to show the existence of a topological state is angle resolved photoelectron spectroscopy (ARPES) where the electronic distribution as a function of momentum is directly observed. A detailed description of ARPES can be found in [10]. When conductance is measured in 3D, it is typically done by placing electrodes on the surface of the material in a 4 probe or Hall geometry.

Prediction, discovery, and other notable publications

In 2007, near the same time as the discovery of the first 2D topological insulator, the first predictions of 3D topologically insulating materials were being published. The earliest predicted 3D topological insulator was $Bi_{1-x}Sb_x$ [4]. The surface states in $Bi_{1-x}Sb_x$ are relatively complex, and in 2009 simpler versions were predicted in Bi_2Te_3 and Sb_2Te_3 [5] as well as Bi_2Se_3[5,6]. Computational results from 2009 for the LDOS of four likely candidates of topological insulators can be seen in Figure 4. In the image it can clearly be seen that, while most of the material is insulating, there are gapless states present.

The first observation of gapless, topologically protected surface states in 3D materials were in 2009 [8,9]. Using ARPES spectra, the existence of such states was shown in Bi_2Te_3, Sb_2Te_3, and Bi_2Se_3. Seen in Figure 5 (image and caption taken from [9]) are the ARPES results in two different planes of a sample of Bi_2Te_3 and at four different doping conditions. The Dirac cone of spin-polarized conductive surface states bridging the gap between the bulk valence and bulk conduction band in Bi_2Te_3 can be seen. The bulk valence band (BVB), bulk conduction band (BCB), and surface state bands (SSB) are depicted. The APRES spectra in the top row are cross sections of the energy vs. momentum graphs in the middle, and the location of the cross-section are indicated by green dotted lines. The experimenters then go on to resolve the 3D band structure by stacking the images, which can be seen in Figure 3 in [9]. Each doping concentration is shifting the Fermi level, and changing where the cross-section is being made relative to the conduction and valence bands.

Another interesting experiment is the emergence of the topologically insulating phase as the sample is increased in thickness from a single quintuple layer (shown in Fig. 7.) to six quintuple layers. The experiment shows the gapless surface states emerge with increasing layers of Bi_2Se_3, which can be seen in Figure 6 as the emergence of states bridging the bulk conduction and valence bands [8]. This result is in good agreement with the idea that the TI state results from bulk properties of the material and is not affected by local variations.

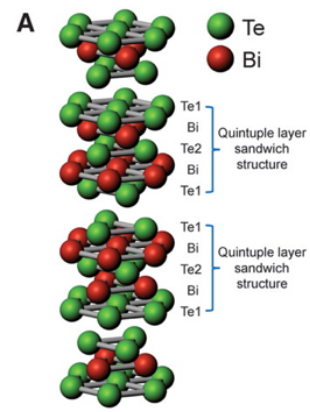


Fig. 7. Crystal structure of Bi_2Te_3, illustrating quintuple layers.

One final 3D topologically insulating material worth mentioning is the verification in 2014 that samarium hexaboride is a topological insulator [13]. It is notable because the material is a known Kondo insulator, which is different from the other the materials mentioned because electrons are strongly correlated in this material. This could lead to novel properties that are distinct from other TIs.

Conclusion

As is hopefully apparent from the discussion in this paper, the field of topological insulators is young and making rapid advances. We can expect in upcoming years that a number of materials which have been predicted to exhibit topologically insulating behavior will be verified. Only a handful of the predicted materials have been experimentally verified. Topological insulators will remain a hot field into the next decade because the intriguing and novel phenomena remains the primary example of protected states without the presence of an external magnetic field. As future generations of integrated circuits evolve, the introduction of dissipation-less transport will be an important step to further scaling down the technology. TIs are ideal materials suited for the task. 2D topological insulators are a much sought after tool for transporting spin polarized current for spin-tronics. Many in the field predict that 3D topological insulators are the key to direct observation of the exotic Majorana fermion, which has eluded detection for many decades. Such a discovery would further cement topological insulators as a major breakthrough in materials physics.

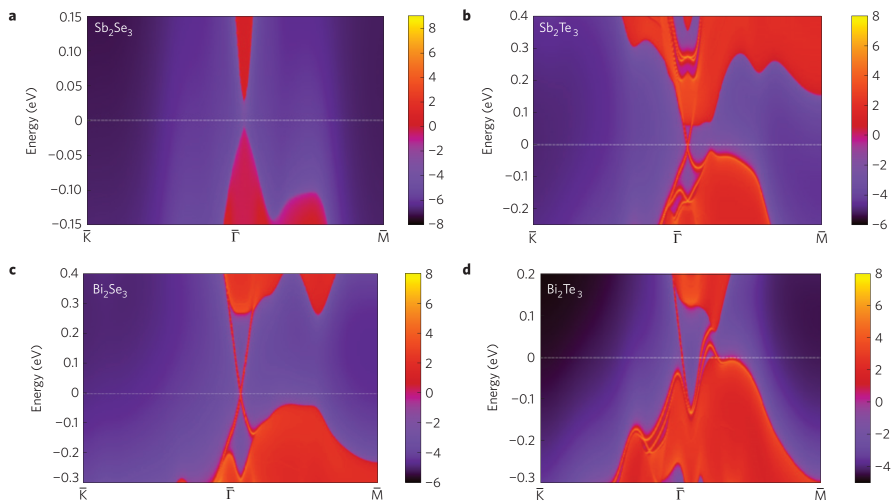


Fig. 4. Energy and momentum dependence of the LDOS for Sb_2Se_3 (a), Sb_2Te_3 (b), Bi_2Se_3 (c) and Bi_2Te_3 (d) on the [111] surface. The red regions indicate bulk energy bands and the blue regions indicate bulk energy gaps. The surface states can be clearly seen around the 0 point as red lines dispersing in the bulk gap. No surface state exists for Sb_2Se_3. Image taken from [5].

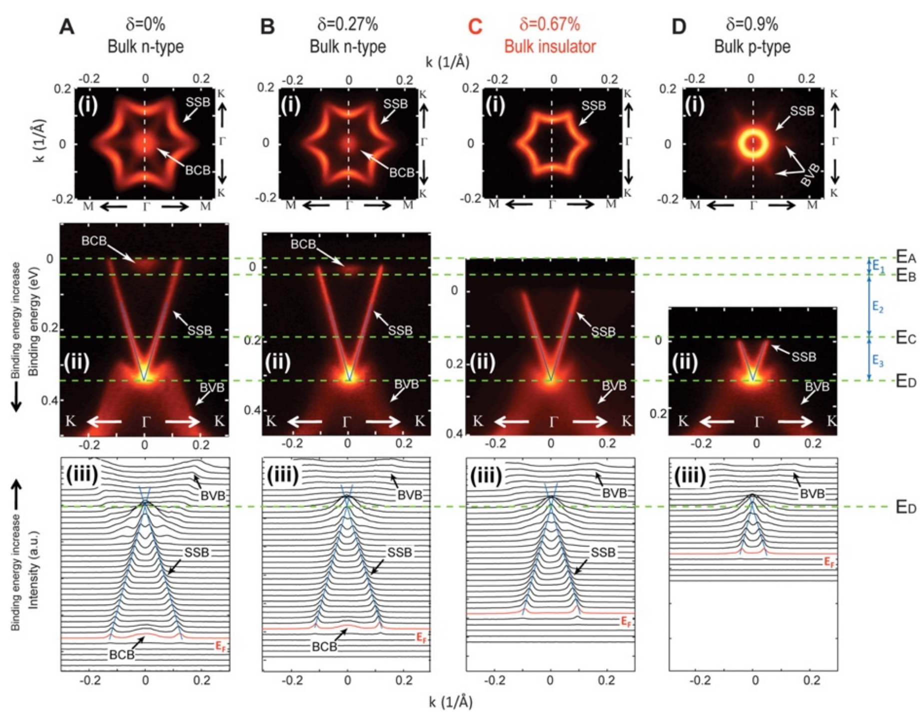


Fig. 5 ARPES spectra of Bi_2Te_3 films at room temperature. Top row: a–d, ARPES spectra of 4 different doping concentrations along the Γ–M direction. They are cross sections of the middle row at the green dashed lines. Middle row: ARPES spectra along the Γ–K direction. Bottom row: Electron density contours. Image taken from [9].

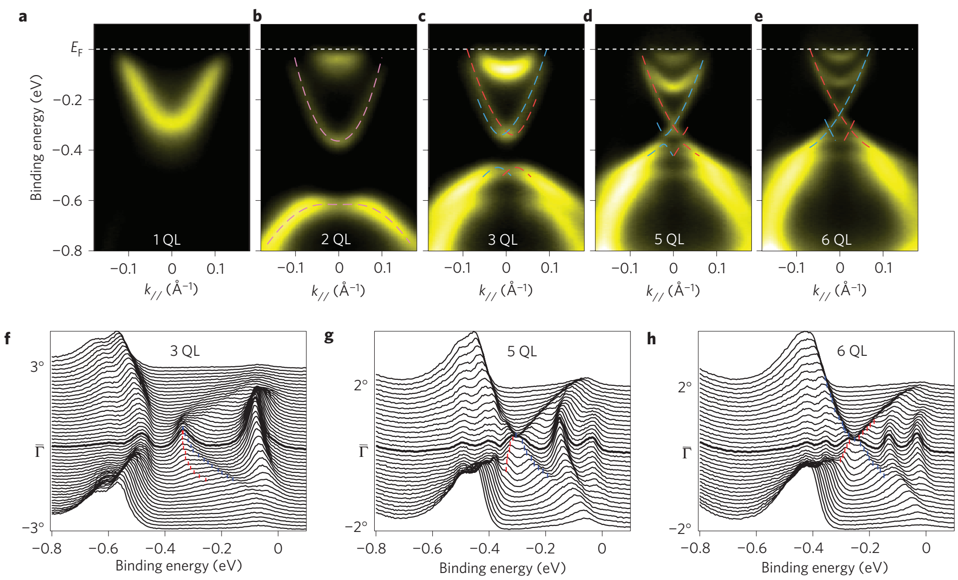


Fig. 6 ARPES spectra of Bi_2Se_3 films at room temperature. Top row: a–e, ARPES spectra of 1 to 6 quintuple layers along the Γ–K direction. Bottom row: Electron density contours. The dashed lines are the fits from equation (1) in [8]. Image taken from [8].

References

[1] Kane, C. L., & Mele, E. J. (2005). Quantum spin Hall effect in graphene.*Physical review letters*, *95*(22), 226801.
[2] Bernevig, B. A., Hughes, T. L., & Zhang, S. C. (2006). Quantum spin Hall effect and topological phase transition in HgTe quantum wells. *Science*,*314*(5806), 1757-1761.
[3] König, M., Wiedmann, S., Brüne, C., Roth, A., Buhmann, H., Molenkamp, L. W., ... & Zhang, S. C. (2007). Quantum spin Hall insulator state in HgTe quantum wells. *Science*, *318*(5851), 766-770.
[4] Fu, L., & Kane, C. L. (2007). Topological insulators with inversion symmetry.*Physical Review B*, *76*(4), 045302.
[5] Zhang, H., Liu, C. X., Qi, X. L., Dai, X., Fang, Z., & Zhang, S. C. (2009). Topological insulators in Bi2Se3, Bi2Te3 and Sb2Te3 with a single Dirac cone on the surface. *Nature physics*, *5*(6), 438-442.
[6] Xia, Y., Qian, D., Hsieh, D., Wray, L., Pal, A., Lin, H., ... & Hasan, M. Z. (2009). Observation of a large-gap topological-insulator class with a single Dirac cone on the surface. *Nature Physics*, *5*(6), 398-402.
[7] Kane, C., & Moore, J. (2011). Topological insulators. *Physics World*, *24*(02), 32.
[8] Zhang, Y., He, K., Chang, C. Z., Song, C. L., Wang, L. L., Chen, X., ... & Shen, S. Q. (2010). Crossover of the three-dimensional topological insulator Bi_2Se_3 to the two-dimensional limit. *Nature Physics*, *6*(8), 584-588.
[9] Chen, Y. L., Analytis, J. G., Chu, J. H., Liu, Z. K., Mo, S. K., Qi, X. L., ... & Zhang, S. C. (2009). Experimental realization of a three-dimensional topological insulator, Bi_2Te_3. *Science*, *325*(5937), 178-181.
[10] Damascelli, A. (2004). Probing the electronic structure of complex systems by ARPES. *Physica Scripta*, *2004*(T109), 61.
[11] Qi, X. L., & Zhang, S. C. (2011). Topological insulators and superconductors. *Reviews of Modern Physics*, *83*(4), 1057.
[12] Fu, L., & Kane, C. L. (2008). Superconducting proximity effect and Majorana fermions at the surface of a topological insulator. *Physical review letters*,*100*(9), 096407.
[13] Kim, D. J., Xia, J., & Fisk, Z. (2013). Topological surface state in the Kondo insulator samarium hexaboride. *arXiv preprint arXiv:1307.0448*.

Resources

[1] Theory Review:
König, M., Buhmann, H., W. Molenkamp, L., Hughes, T., Liu, C. X., Qi, X. L., & Zhang, S. C. (2008). The quantum spin Hall effect: theory and experiment.*Journal of the Physical Society of Japan*, *77*(3), 031007.
[2] Short review:
Kane, C., & Moore, J. (2011). Topological insulators. *Physics World*, *24*(02), 32.
[3] General review of Topological Insulators and Superconductors:
Qi, X. L., & Zhang, S. C. (2011). Topological insulators and superconductors.*Reviews of Modern Physics*, *83*(4), 1057.
[4] Nature perspective article: Moore, J. E. (2010). The birth of topological insulators. *Nature*, *464*(7286), 194-198.