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. Some common examples are magnets, which break rotational symmetry, superconductors, which break

Topological Insulators (and topologically protected states in general) are a state of matter of particular interest because they deviate from this general description of phases and symmetries. 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 do not possess this property and the universe as a whole does not.

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.

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 time-reversal (TR) symmetry and that there is a strong strong 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 state discovered to exhibit a topologically protected state is 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 was quantized at integer values of e²/h independent of sample quality and size. The term *topological invariant* has become a useful concept. It describes a quantity like the Hall conductance that is invariant under small changes in the material. They often take the form of an integral which is invariant and depends only on the most general properties of the system, but whose integrand may vary. In the case of topological invariant is an integral of Bloch wave functions over momentum space.

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



(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 romotion 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.

momentum plays the role 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. 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.

Displayed in Figure 1d is an analogy of how this effect generalizes into three dimensions, where surface states move in the direction of $G = 0.01 e^2/h$ 20 ш their spin. A gapless Dirac cone of surface 10 15 ĝ R_{14,23}// states is formed connecting the bulk valence 10 T = 30 mK 10⁶ 5 $R_{14,23} / \Omega$ and conduction bands. This is discussed -0.5 0.0 1.0 10⁵ further in the 3D topological insulator theory

Prediction and discovery

section.

In a somewhat unusual fashion for condensed matter physics, the 2D topological 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 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. Further evidence is seen in the destruction of the state though application of a magnetic field is seen in Figure 3, where the conductance



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]



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 $(L \times \Omega) = (20 \times \Omega)$ 13.3) μ m² measured in a vector field cryostat at 1.4 K. Image and caption taken from [3]

goes to zero with increasing magnetic field perpendicular to the plane of the material.

3D Topological Insulators

Theory

Generalizing the phenomena of topological insulators to 3D is messy, and the early predictions of such states were complicated. The models continue 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.

In two dimensions the 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 is a two dimensional surface of states who conduct in the direction of their spin. It is illustrated in a band diagram as a cone of topologically protected states connecting the bulk valence and conduction band states.

Measuring a state near OK with conductance quantized in units of e²/h, independent of sample width is convincing evidence of a 2D topological insulator. However, experimental detection of the 3D topologically insulating state is more difficult because the conductance isn't expected to be precisely zero near OK. The technique used is angle resolved photoelectron spectroscopy (ARPES) to directly observe the electronic distribution.

Prediction and discovery

In 2007, near the same time of the discovery of the first 2D topological insulator, the first predictions of 3D topologically insulating materials were being published, predicting several materials to exhibit the behavior, the earliest of which was $Bi_{1-x}Sb_x$ [4]. In 2009, simpler versions were then predicted in Bi_2Te_3 and Sb_2Te_3 [5] as well Bi_2Se_3 [5,6]. The 2009 results for the LDOS of the surface states can be seen in Figure 4.

Conductive, topologically protected surface states in these later three materials were first observed in 2009 as well [7,8]. Seen in Figure 5 (image and caption taken from [7]) is the ARPES results in two different planes showing the Dirac cone of conductive surface states bridging the gap between the bulk valence and bulk conduction band in .



Fig. 4. Energy and momentum dependence of the LDOS for Sb₂Se₃ (a), Sb₂Te₃ (b), Bi₂Se₃ (c) and Bi₂Te₃ (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 Sb₂Se₃.





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 $\Gamma-K$ direction. Bottom row: Energy density contours. The dashed lines are the fits from equation (1) in [8]. Image taken from [8].

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