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THE NEW STATE OF MATTER - TOPOLOGICAL INSULATORS AND QUANTUM PHASE TRANSITION

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ABSTRACT

An overview of the basic concepts of topological insulators and recent studies of these remark-able new materials. They are characterized by a full insulating gap in the bulk and gapless edge or surface states which are protected by time-reversal symmetry. These topological materials have been theoretically predicted and experimentally observed in a variety of systems, including HgTe quantum wells, BiSb alloys, and Bi_2Te_3 and Bi_2Se_3 crystals. I discuss recent advances made in the study of topological insulators for both bulk and nanostructured materials and in the theoretical understanding of these materials. Some insulators have unusual metallic states on their surfaces. These states are formed by topological effects that also render the electrons travelling on such surfaces insensitive to scattering by impurities. Such topological insulators may provide new routes to generating new phases and particles, possibly finding uses in technological applications.

Keywords : Topological insulators, Spin orbit coupling, topological field theory, Quantum Hall state and topological phases.

I. INTRODUCTION

The greatest achievement of condensed matter physics in the last century is the classification of these quantum states by the principle of spontaneous symmetry breaking[1]. In 1980, a new quantum state was discovered which does not fit into this simple paradigm[2] called as the quantum Hall (QH) state, the bulk of the two-dimensional (2D) sample is insulating, and the electric current is carried only along the edge of the sample. The flow of this unidirectional current avoids dissipation and gives rise to a quantized Hall effect. The QH state provided the first example of a quantum state which is topologically distinct from all states of matter known before. In mathematics, topological classification discards small details and focuses on the fundamental distinction of shapes. In physics, one can consider general Hamiltonians of many-particle systems with an energy gap separating the ground state from the excited states. In this case, one can define a smooth deformation as a change in the Hamiltonian which does not close the bulk gap. This topological concept can be applied to both insulators and superconductors with a full energy gap, which are the focus of this article. The abstract concept of topological classification can be applied to condensed matter system with an energy gap, where the notion of a smooth deformation can be defined[3]. Further progress can be made through the concepts of topological order parameter and topological field theory (TFT), which are powerful tools describing topological states of quantum matter. The QH states belong to a topological class which explicitly breaks time-reversal (TR) symmetry, for example, by the presence of a magnetic field. In recent years, a new topological class of materials has been theoretically predicted and experimentally observed[4-9]. These new quantum states belong to a class which is invariant under TR, and where spin-orbit coupling (SOC) plays an essential role. All TR invariant insulators in nature fall into two distinct classes, classified by a Z_2 topological order parameter. The topologically nontrivial state has a full insulating gap in the bulk, but has gapless edge or surface states consisting of an odd number of Dirac fermions. The topological property manifests itself more dramatically when TR symmetry is preserved in the bulk but broken on the surface, in which case the material is fully insulating both inside the bulk and on the surface. In this case, Maxwell's laws of electrodynamics are dramatically altered by a topological term with a precisely quantized coefficient, similar to the case of the QH effect. The discovery of topologic al insulators has undoubtedly had a dramatic impact on the field of condensed matter physics.

II. TWO-DIMENSIONAL TOPOLOGICAL INSULATORS

The Quantum Spin Hall (QSH) state, or the 2D topological insulator was first discovered in the HgTe/CdTe quantum wells. Bernevig, Hughes and Zhang[10] initiated the search for the QSH state in semiconductors with an “inverted” electronic gap, and predicted a quantum phase transition in HgTe/CdTe quantum wells as a function of the thickness of the quantum well. The general mechanism is band inversion, in which the usual ordering of the conduction band valence band is inverted by spin-orbit coupling[11,12]. In certain heavy elements such as Hg and Te, the spin-orbit coupling is so large that the p-orbital band is pushed above the s-orbital band that is, the bands are inverted. Mercury telluride quantum wells can be prepared by sandwiching the material between cadmium telluride, which has a similar lattice constant but much weaker spin-orbit coupling. Therefore, increasing the thickness d of the HgTe layer increases the strength of the spin-orbit coupling for the entire quantum well. The behavior of a mercury telluride-cadmium telluride quantum well depends on the thickness d of the of the HgTe layer. For a thin quantum well, as shown in the left column of figure 1a, the CdTe has the dominant effect and the bands have a normal ordering: The s-like conduction subband E1 is located above the p-like valence subband H1. In a thick quantum well, as shown in the right column, the opposite ordering occurs due to increased thickness d of the HgTe layer. The critical thickness d_c for band inversion is predicted to be around 6.5 nm. The QSH state in HgTe can be described by a simple model for the E1 and H1 subbands. Explicit solution of that model gives one pair of edge states for $d > d_c$ in the inverted regime and no edge states in the $d < d_c$, as shown in figure 1b. The pair of edge states carry opposite spins and disperse all the way from valence band to conduction band. The crossing of the dispersion curves is required by TR symmetry and cannot be removed it is one of the topological signatures of a QSH insulator. A sharp conductance difference between thin and thick quantum wells was observed experimentally, as shown in figure 1c.

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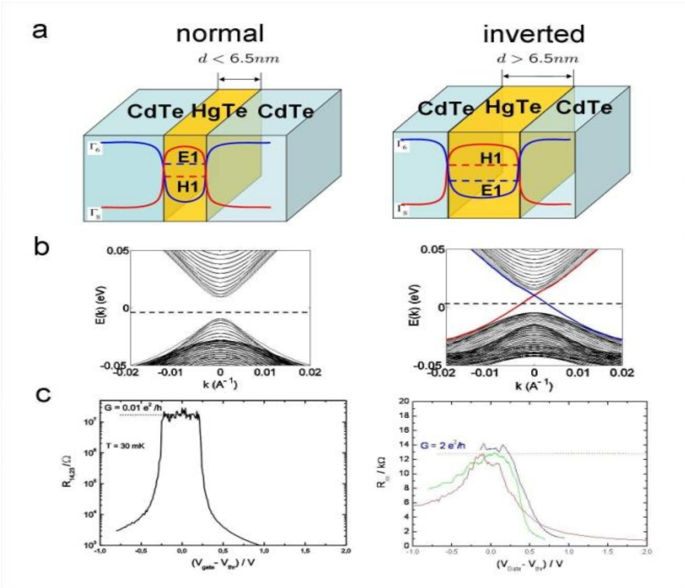
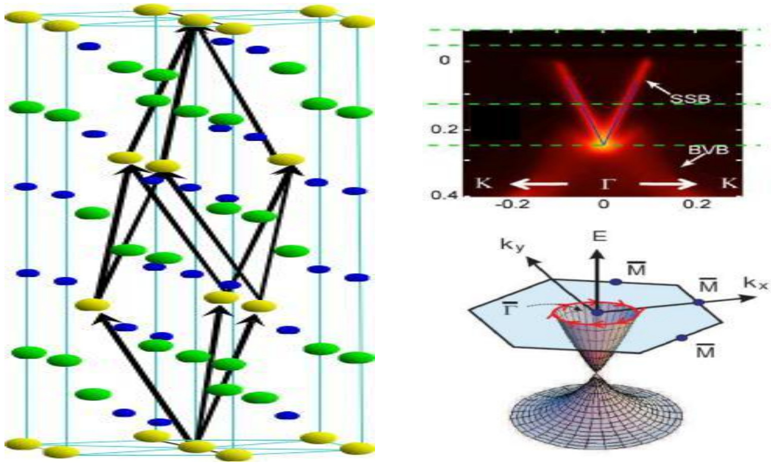


Fig.1

III. THREE-DIMENSIONAL TOPOLOGICAL INSULATOR

From figure 3b we see that the 2D topological insulator has a pair of 1D edge states crossing at momentum k = 0. Near the crossing point, the dispersion of the states is linear. That's exactly the dispersion one gets in quantum field theory from the Dirac equation for a massless relativistic fermion in 1D, and thus that equation can be used to describe the QSH edge state. Such a picture can be simply generalized to a 3D topological insulator, for which the surface state consists of a single 2D massless Dirac fermion and the dispersion forms a so-called Dirac cone, as illustrated in figure 2. Similar to the 2D case, the crossing point the tip of the cone is located at a TR-invariant point, such as at k = 0, and the degeneracy is protected by TR symmetry. The Zhong Fangs group at the Chinese Academy of Sciences, predicted that Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3, all with the layered structure in figure 2a, are 3D topological insulators, whereas a related material, Sb_2Se_3, is not[13] . As in HgTe, the nontrivial topology of the Bi_2Te_3 family is due to band inversion between two orbitals with opposite parity, driven by the strong spin-orbit coupling of Bi and Te. First-principle calculations show that the materials have a single Dirac cone on the surface. The spin of the surface state lies in the surface plane and is always perpendicular to the momentum, as shown in figure 2b. The observed surface states indeed disperse linearly, crossing at the point with zero momentum as shown in figure 2c.

a. b.



F. Other topological insulator materials

The topological materials HgTe, Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3 not only provide us with a prototype material for 2D and 3D topological insulators, but also give us a rule of thumb to search for new topological insulator materials. The non-trivial topological property of topological insulators originates from the inverted band structure induced by SOC. Therefore, it is more likely to find topological insulators in materials which consist of covalent compounds with narrow band gaps and heavy atoms with strong SOC. Following such a guiding principle, a large number of topological insulator materials have been proposed recently, which can be roughly classified into several different groups as shown in Table 1.

Table I. Proposed topological insulator materials grouped into several different material classes.[4,12,13,19,23–29]

HgTe-type	Bi_2Se_3-type	Honey Comb Lattice	Bismuth-Alloys	NaCl Structure	Oxides	Correlated Materials	Super-conductors
HgTe	Bi_2Se_3, Bi_2Te_3, and Sb_2Te3	Graphene	Bi-Sb	SnTe PbTe	Doped $BaBiO_3$	Iridates	$Cu_xBi_2Se_3$
Half-Heuslers such as LaPtBi	Bi_2Te_2Se	LiAuTe		PuTe AmN	Iridates	SmB_6	LaPtBi YPtBi LuPtBi
α-Sn, HgSe β-HgS	$(Bi_xSb_{1-x})_2Te_3$					YbPtBi	$TlBiSe_2$ $TlBiTe_2$
Chalco-pyrites	$TlBiSe_2$ and $TlBiTe_2$					Skutterudites	
AlSb/InAs/GaSb	$Bi_{14}Rh_3I_9$					PuTe, AmN	

Table 1

The first group is similar to the tetradymite semiconductors, where the atomic p-orbitals of Bi or Sb play an essential role. Thallium-based III-V-VI_2 ternary chalcogenides, including $TlBiQ_2$ and $TlSbQ_2$ with Q = Te, Se and S, belong to this class[14]. These materials have the same rhombohedral crystal structure (space group D^5) as contrast to the layered tetradymite compounds. These materials have recently been experimentally observed to be topological insulator[15,16]. A typical material of the second group is distorted bulk HgTe. In contrast to conventional zincblende semiconductors, HgTe has an inverted bulk band structure. A similar band structure also exists in ternary Heusler compounds[17,18], and around fifty of them are found to exhibit band in-version.

These materials become 3D topological insulators upon distortion, or they can be grown in quantum well form similar to HgTe/CdTe to realize the 2D or the QSH insulators. Due to the diversity of Heusler materials, multifunctional topological insulators can be realized with additional properties ranging from superconductivity to magnetism and heavy-fermion behavior. There are also some other theoretical proposals of new topological insulator materials with electron correlation effects. An example is the case of Ir-based materials. The QSH effect has been proposed in Na_2IrO_3[19] and topological Mott insulator phases have been proposed in Ir-based pyrochlore oxides $Ln_2Ir_2O_7$ with Ln = Nd, Pr[20-23].

IV. THEORY OF TOPOLOGICAL INSULATORS

Topological materials in general, and topological insulators in particular, can be defined by physically measurable topological invariants in topological field theories. We can first divide insulators into two broad classes, according to the presence or absence of TR symmetry. The QH state is a topological insulator state that breaks TR symmetry. David Thouless and coworkers showed that the physically measured integer QH conductance is given by a topological invariant called the first Chern number. For a generally interacting system, the topological properties of the QH state can be described by an effective topological field theory based on the ChernCSimons theor[24]. Although Duncan Haldane constructed a model of the QH effect without the external magnetic field, that state still breaks TR symmetry. For a long time it was widely believed that both TR symmetry breaking and two dimensionality are necessary for an insulator to be topological, but in 2001 the first model of a TR-invariant topological insulator was introduce[25]. That model was originally defined in 4D, but TR-invariant topological insulators in 3D and 2D can be obtained through a simple dimension-reduction procedure[26] Shuichi Murakami, Naoto Nagaosa, and Zhang, and in parallel MacDonald and colleagues at the

University of Texas in Austin, developed the theory of the intrinsic spin Hall effect in doped semiconductors and identified spin-orbit coupling as the crucial ingredient; later, Murakami, Nagaosa, and Zhang extended the theory to TR-invariant insulators. Kane and Mele first introduced the topological band theory of TR-invariant QSH insulators in 2D and showed that they fall into two distinct topological classes, generally referred to as the Z_2 classification [27]. This topological band theory was soon generalized to three dimensions [28]. We now have two precise definitions of TR-invariant topological insulators, one in terms of noninteracting topological band theory and one in terms of topological field theory. If we approximate an insulator with nonin-teracting electrons filling a certain number of bands, the topological band theory can evaluate an explicit topological invariant that can give only binary values of 0 or 1: a Z_2 classification that defines trivial and nontrivial insulators. For materials with inversion symmetry, a powerful algorithm developed by Fu and Kane [29] can be easily integrated into electronic structure calculations to numerically evaluate the topological band invariant. Since all insulators in nature are necessarily interacting, it is important to have a general definition of topological insulators that is valid for interacting systems and is experimentally measurable. Both problems were solved with the topological field theory which can be generally defined for all insulators, with or without interactions.

V. CONCLUSION

The subject of topological insulators and topological superconductors is now one of the most active fields of research in condensed matter physics, developing at a rapid pace. Theorists have systematically classified topological states in all dimensions. For future progress on the theoretical side, the most important outstanding problems include interaction and disorder effects, realistic predictions for topological Mott insulator materials, a deeper understanding of fractional topological insulators and realistic predictions for materials realizations of such states, the effective field theory description of the topological superconducting state, and realistic materials predictions for topological superconductors. On the experimental part, the most important task is to grow materials with sufficient purity so that the bulk insulating behavior can be reached, and to tune the Fermi level close to the Dirac point of the surface state.

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