Topological Insulator: A new state of matter with new promises

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1 Topological state in condensed matter

The conventional way of viewing the phases/states in condensed matter is from the point of broken/enhanced symmetry, e.g. crystals with broken translational and rotational symmetry, ferromagnets with broken rotational and time-reversal symmetry, and superconductors with broken U(1) gauge symmetry. However, after the discovery of quantum hall effect (QHE) [1], though not understood at that time, the perception about states of matter has moved from symmetry broken order to a different kind of order, reasonably termed as the topological order. One may argue that QHE arises in 2D electron gas by applying magnetic field that breaks time-reversal (TR) symmetry of the system and hence can be viewed as a result of broken TR symmetry. However, the topological connection has been discussed in the next section and the recent realization of the quantum spin Hall effect (QSHE) due to presence of strong spin-orbit (SO) coupling, which is a relativistic effect that preserves the TR symmetry, forces us think of a new state of matter. This new material is like a band insulator in the bulk with protected (unaffected by disorder) conducting states on the edges or surfaces and hence it is named topological insulator. Presence of this protected state has drawn a big attention to the scientific community with a promise of dissipationless modern computation. The topological order concept was first introduced in the context of fractional quantum Hall effect by X-G Wen in 1995 [2].

2 Topological order in 2D, topological invariants

2.1 TKNN invariant

The QHE shows a quantized conductivity :

$$\sigma_{xy} = n\frac{e^2}{h} \tag{1}$$

Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) [3] identified this integer n as an integral of the Bloch wave functions over the magnetic Brillouin zone (BZ), and corresponds to the first Chern class of a $U(1)$ principal fiber bundle on a torus. The periodicity of a crystal Hamiltonian can be topologically mapped onto a torus. A torus or band-structures are topologically equivalent if the former can be deformed to the latter continuously without closing the bandgap. Thus they both share the same topological invariant, which is denoted by n, the Chern number. The Chern number is the Euler characteristic that appears as an integer in the Gauss-Bonnet theorem in Riemann manifold. The Chern number can be associated to the Berry phase which appears in the Bloch wave function $|u_m(\mathbf{k})\rangle$ when its momentum $\mathbf{k}$ in the band m moves around the closed loop of a periodic BZ. The Berry phase is given in form of a line integral $\mathcal{A}_m = i\langle u_m|\nabla_k|u_m\rangle$ which can be finally written in term of Berry flux $\mathcal{F}_m = \nabla \times \mathcal{A}_m$ and the Chern number will be

$$n = \sum_m \frac{1}{2\pi} \int d^2\mathbf{k}\, \mathcal{F}_m \tag{2}$$

TKNN showed the conductivity σ_{xy} calculated from the Kubo formula has the same form and hence the Chern number is exactly the same in both cases.

2.2 Z_2 invariant

Now as we know that the QHE appears only when the TR is broken, the Hall conductivity and hence the TKNN invariant $n = 0$ when there is a TR symmetry. As we mentioned before that in QSHE, though there will be two Chern numbers $n_\uparrow$ and $n_\downarrow$, the total number $n = n_\uparrow + n_\downarrow = 0$ due to the presence of TR symmetry, whereas the Hall conductivity for spins will be finite and quantized since $n_\uparrow$ - $n_\downarrow \neq 0$ (i.e. S_z is conserved). This spin conservation and hence Hall quantization can break down in presence of other interactions or disorder, but the topological order will not be disturbed since Kramer's theorem for the spin-$\frac{1}{2}$ particles protects the edge states [4, 5, 6]. The presence of protected edge state even when TKKN invariant $n = 0$ distinguishes from ordinary insulator and offers a new class of topological invariant, which is classified as Z_2 topological order. This additional invariant can have two possible values, $\nu = 0$ (trivial insulator) and $\nu = 1$ (topological insulator). By simple arguments based on Haldane model Kane and Mele [7] showed that the quantum spin Hall insulator (QSHI) is robust only when number of edge states crossing the Fermi level is odd, the Z_2 number is $\nu = 1$. When the number of edge states is even it becomes a trivial insulator ($\nu = 0$).

3 Topological order in 3D

Since there is no QHE in 3D, the only way to get a 3D TI is through layers of 2D QSHIs. However, Moore and Balent [6] showed that apart from three invariants coming from three layers, another fourth Z_2 invariant exists. Therefore total $2^4 = 16$ different classes of TI can emerge. Thus the Z_2 invariants are written as $\nu_0; \nu_1, \nu_2, \nu_3$. The layered 3D insulator ($\nu_0 = 0$) is termed as the weak topological insulator (WTI) since presence of disorder can localize the surface states and the insulator becomes equivalent to a band insulator. In contrast, $\nu_0 = 1$ for the strong topological insulators (STI), one can think of a Dirac cone with Kramers degeneracy at the Dirac point. The surface of a STI forms a 2D topological metal that encloses odd number of such Dirac points.

4 Experimental realization

4.1 2D TI

Though spin-orbit interaction exists in all materials, only a few turned out to be suitable candidates for 2D TI. In 2006, Berenvig, Hughes, and Zhang [8] proposed that such a QSHI state can be realized in HgTe quantum well structure sandwiched between CdTe. Their prediction was based on the theory of band inversion that arise due to the strong SO coupling that affects beyond a critical thickness of HgTe layer. In a short while a team led by Laurens Molenkamp [9] from the university of Würzburg observed the QSH effect in HgTe quantum wells grown by molecular beam epitaxy. Since the QSHI with TR symmetry does not promise QHE, they found only the mesoscopic Landauer-Büttiker [10] conductance, i.e. $\sigma = 2e^2/h$ from the edge states.

4.2 3D TI

Zhang's group's calculation shows that the dispersion relation for the edge states in 2D TI is linear which is exactly a characteristic of massless Dirac fermions. If this can be generalized to 3D then one should expect a Dirac cone. Fu and Kane [11] estimated the Z_2 invariants from the knowledge of the parity of the TR invariant momenta Γ_i in the BZ. Based on their calculation they predicted that the alloy $Bi_{1-x}Sb_x$ and α-Sn and HgTe under uniaxial strain could be good candidates for STI. Zahid Hasan's group [12] first found topological surface states (Dirac cone) in $Bi_{1-x}Sb_x$ alloy. The search moved forward to other materials, e.g. Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 following later prediction by Zhang's group [13]. Further STM and spin-ARPES measurement on Bi_2Se_3 samples by Robert Cava's group [14] in collaboration with Hasan's group confirmed that the spins indeed lie on the surface where backscattering is found to be absent despite strong atomic scale disorder.

5 Applications

5.1 Axion electrodynamics

In electromagnetic field theory the Lagrangian density can be written as

$$\mathcal{L}_0 = \frac{1}{8\pi}(\epsilon \mathbf{E}^2 - \frac{1}{\mu}\mathbf{B}^2)\,. \tag{3}$$

Now the question arises: what happen when we have electro-magnetic coupling, i.e. an additional term

$$\mathcal{L}_\theta = \frac{\theta e^2}{2\pi h}\mathbf{E}.\mathbf{B} = \frac{\theta e^2}{16\pi h}\epsilon^{\mu\nu\lambda\delta}F_{\mu\nu}F_{\lambda\delta} = \frac{\theta e^2}{8\pi h}\epsilon^{\mu\nu\lambda\delta}\partial_\mu(A_\nu F_{\lambda\delta}) \tag{4}$$

arises with invariance under $\theta \to \theta + 2\pi$. This additional term is known as the axion field term which has been introduced in order to solve strong CP violation problem in particle physics [16, 15]. Since $\mathbf{E}$ is TR invariant and $\mathbf{B}$ is odd to TR symmetry, the Lagrangian loses the TR symmetry unless θ is odd to TR as well. Now Qi *et al.* [17] and Essine, Moore and Vanderbilt [18] argued that the trivial TI and STI belong to the special choices of $\theta = 0$ and $\theta = \pi$ respectively. Hence they belong to the Z_2 invariant class and θ/π is identical to the invariant ν_0. This particular choice of θ arises due to its periodicity over 2π and can be understood from the analogy with magnetic field in a 1-D ring where the electron wavefunction picks up a phase depending on two special choices of the magnetic flux $\Phi = 0$ or $\Phi = hc/(2e)$ after completing a full circular path. According to the topological field theory the coefficient in the axion term (after the second equality in the above eq.) gives the value of the Hall conductance [19]. Thus $\theta = \pi$ gives rise to $1/2(e^2/h)$ which can only be shifted by an integer due to disorders. This measurement of surface Hall conductivity in STI can become a confirmation topological robustness and the axion electrodynamics as well.

5.2 Majorana fermions

Majorana fermion is a fermion which is its own antiparticle. A particle to be its own particle is true for spin-1 photon and spin-0 neutral pions. However, this has not been yet observed in any known half-spin integral particle. Majorana fermion state appears when the Dirac equation is treated for real field solutions instead of complex field for electrons/positrons [20]. The possibility for Majorana particle is first thought for the neutral neutrino or anti-neutrino and the double-beta decay is being quested for a long time. The other possibility is in the supersymmetry partner of neutral bosonic fields, e.g. the superpartner photino for photons, may be confirmed in recent large hadron collider (LHC) experiment going on in CERN, Geneva.

Jackiw with Rebbi [21] and Rossi [22] showed that, apart from the positive an negative energy eigen values, a bound isolated zero energy mode can exist with a Dirac-type equation in presence of a topological defect, e.g. soliton/domain wall in polyacetylene (1D), vortex in a 2D superconductor, and 't Hooft magnetic monopole in 3D. In case of conventional Dirac representation this zero mode gives rise to charge fractionalization ($\pm 1/2$), whereas in Majorana representation [20] that treats the field operator to be real, zero mode with chargeless (neutral) Majorana fermion emerges.

Realization of such bound Majorana states (MBS) is first proposed by Read and Green [23] for the $p_x + ip_y$ wave superconductor, e.g. in Sr_2RuO_4 [24] and in cold-atoms [25]. They found that the Bogolioubov-de Genes (BdG) equation for weak pairing superconductor can be deduced to Dirac equation with real fields and presence of vortex leads to bound Majorana state. Though conventional s-wave superconductor does not show zero modes, the presence of MBS can be found in topological superconductors which can arise in a strong TI due to proximity effect when the TI's surface is close to that of a superconductor. Fu an Kane [26] suggested some methods to engineer them in real experiments.

5.3 Next generation computer

The protected surface/edge states promise to get rid of decoherence in the spin current which is very crucial for next generation quantum computation. Also if bound Majorana fermions ever been found, their non-Abelian statistics will build the qubits necessary for quantum calculation [27].

6 Open challenges

Despite my short-term visit through literature, I believe the following issues still persist.

6.1 Experimental

1. More and efficient TIs, specially with large band gap in the bulk without mixing to the edge/surface states.
2. Measure magnetoelectric effect.
3. Optimize proximity effect.
4. Suitable superconductor which makes good interfaces.
5. Create and detect Majorana bound states.

6.2 Theoretical

1. Theory for protected edge states considering interaction.
2. Effect of disorder and interaction.
3. Effect of superconductivity.
4. Role of topological defects (e.g. dislocation [28]).
5. Predict other TIs.
6. Enhance figure of merit in thermoelectric TIs [29].

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