The quantum spin Hall effect and topological insulators
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In the quantum world, atoms and their electrons can form many different states of matter, such as crystalline solids, magnets, and superconductors. Those different states can be classified by the symmetries they spontaneously break—translational, rotational, and gauge symmetries, respectively, for the examples above. Before 1980 all states of matter in condensed-matter systems could be classified by the principle of broken symmetry. The quantum Hall (QH) state, discovered in 1980, provided the first example of a quantum state that has no spontaneously broken symmetry. Its behavior depends only on its topology and not on its specific geometry; it was topologically distinct from all previously known states of matter.

Recently, a new class of topological states has emerged, called quantum spin Hall (QSH) states or topological insulators (see PHYSICS TODAY, January 2008, page 19). Topologically distinct from all other known states of matter, including QH states, QSH states have been theoretically predicted and experimentally observed in mercury telluride quantum wells, in bismuth antimony alloys, and in Bi$_2$Se$_3$ and Bi$_2$Te$_3$ bulk crystals. QSH systems are insulating in the bulk—they have an energy gap separating the valence and conduction bands—but on the boundary they have gapless edge or surface states that are topologically protected and immune to impurities or geometric perturbations. Inside such a topological insulator, Maxwell’s laws of electromagnetism are dramatically altered by an additional topological term with a precisely quantized coefficient, which gives rise to remarkable physical effects. Whereas the QSH state shares many similarities with the QH state, it differs in important ways. In particular, QH states require an external magnetic field, which breaks time-reversal (TR) symmetry; QSH states, in contrast, are TR invariant and do not require an applied field.

In topological insulators, spin–orbit coupling and time-reversal symmetry combine to form a novel state of matter predicted to have exotic physical properties.

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Figure 1. Spatial separation is at the heart of both the quantum Hall (QH) and the quantum spin Hall (QSH) effects. (a) A spinless one-dimensional system has both a forward and a backward mover. Those two basic degrees of freedom are spatially separated in a QH bar, as illustrated by the symbolic equation “$2 = 1 + 1$.” The upper edge contains only a forward mover and the lower edge has only a backward mover. The states are robust: They will go around an impurity without scattering. (b) A spinful 1D system has four basic channels, which are spatially separated in a QSH bar: The upper edge contains a forward mover with up spin and a backward mover with down spin, and conversely for the lower edge. That separation is illustrated by the symbolic equation “$4 = 2 + 2$.”

From quantum Hall to quantum spin Hall

In a one-dimensional world, there are two basic motions: forward and backward. Random scattering can cause them to mix, which leads to resistance. Just as we have learned from basic traffic control, it would be much better if we could spatially separate the counterflow directions into two separate lanes, so that random collisions could be easily avoided. That simple traffic control mechanism turns out to be the essence of the QH effect. The QH effect occurs when a strong magnetic field is applied to a 2D gas of electrons in a semiconductor. At low temperature and high magnetic field, electrons travel only along the edge of the semiconductor, and the two counterflows of electrons are spatially separated into different “lanes” located at the sample’s top and bottom edges. Compared with a 1D system with electrons propagating in both directions, the top edge of a QH bar contains only half the degrees of freedom. That unique spatial separation is illustrated in figure 1a by the symbolic equation “$2 = 1$ [forward mover] + 1 [backward mover]” and is the key reason why the QH effect is topologically robust. When an edge-state electron encounters an impurity, it simply takes a detour and still keeps going in the same direction (figure 1), as there is no way for it to turn
back. Such a dissipationless transport mechanism could be extremely useful for semiconductor devices. Unfortunately, the requirement of a large magnetic field severely limits the application potential of the QH effect.

Can we get rid of the magnetic field and still separate the traffic lanes for the electrons? In a real 1D system, forward- and backward-moving channels for both spin-up and spin-down electrons give rise to four channels, as shown in figure 1b. The traffic lanes for the electrons can be split in a TR-invariant fashion, without any magnetic field, as illustrated in the figure by the symbolic equation “4 = 2 + 2.” We can leave the spin-up forward mover and the spin-down backward mover on the top edge and move the other two channels to the bottom edge. A system with such edge states is said to be in a QSH state, because it has a net transport of spin forward along the top edge and backward along the bottom edge, just like the separated transport of charge in the QH state. Charles Kane and Eugene Mele from the University of Pennsylvania, and Andrei Bernevig and one of us (Zhang) from Stanford University, independently proposed in 2005 and 2006 that such a separation, and thus the QSH state, can in principle be realized in certain theoretical models with spin–orbit coupling. (The fractional QSH state was also predicted, though it has yet to be experimentally observed.)

Although a QSH edge consists of both backward and forward movers, backscattering by nonmagnetic impurities is forbidden. To understand that effect, we start with an analogy from daily life. Most eyeglasses and camera lenses have a so-called antireflection coating. As shown in figure 2a, reflected light from the top and the bottom surfaces interfere with each other destructively, leading to zero net reflection and thus perfect transmission. However, such an effect is not robust, as it depends on the matching between the optical wavelength and the thickness of the coating.

Just like the reflection of a photon by a surface, an electron can be reflected by an impurity, and different reflection paths also interfere with each other. As shown in figure 2b, an electron in a QSH edge state can take either a clockwise or a counterclockwise turn around the impurity, and during that turn the spin rotates by an angle of $\pi$ or $-\pi$ to the opposite direction. Consequently, the two paths, related by TR symmetry, differ by a full $\pi - (-\pi) = 2\pi$ rotation of the electron spin. A profound and yet deeply mysterious principle of quantum mechanics states that the wavefunction of a spin-$\frac{1}{2}$ particle obtains a negative sign upon a full $2\pi$ rotation. Thus the two backscattering paths always interfere destructively, which leads to perfect transmission. If the impurity carries a magnetic moment, the TR symmetry is broken and the two reflected waves no longer interfere destructively. In that sense the robustness of the QSH edge state is protected by the TR symmetry.

The physical picture above applies only to the case of single pairs of QSH edge states. If there are two forward movers and two backward movers in the system—as, for example, the unseparated 1D system shown in figure 1b—then an electron can be scattered from a forward-to a backward-moving channel without reversing its spin and without the perfect destructive interference, and thus there is dissipation. Consequently, for the QSH state to be robust, the edge states must consist of an odd number of forward movers and an odd number of backward movers. That even–odd effect, characterized by a so-called $Z_2$ topological quantum number, is at the heart of the QSH state and is why a QSH insulator is also synonymously referred to as a topological insulator.

Two-dimensional topological insulators

Looking at figure 1b, we see that the QSH effect requires the counterpropagation of opposite spin states. Such a coupling between the spin and the orbital motion is a relativistic effect most pronounced in heavy elements. Although all materials have spin–orbit coupling, only a few of them turn out to be topological insulators. In 2006 Bernevig, Taylor Hughes, and Zhang proposed a general mechanism for finding topological insulators and predicted in particular that mercury telluride quantum wells—nanoscopic layers sandwiched between other materials—are topological insulators beyond a critical thickness $d_c$. The general mechanism is band inversion, in which the usual ordering of the conduction band and valence band is inverted by spin–orbit coupling.

In most common semiconductors, the conduction band is formed from electrons in s orbitals and the valence band is formed from electrons in p orbitals. In certain heavy elements such as Hg and Te, however, 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. For a thin quantum well, as shown in the left column of figure 3a, the CdTe has the dominant effect and the bands are inverted by spin–orbit coupling.

Figure 2. (a) On a lens with antireflection coating, light waves reflected by the top (blue line) and the bottom (red line) surfaces interfere destructively, which leads to suppressed reflection. (b) A quantum spin Hall edge state can be scattered in two directions by a nonmagnetic impurity. Going clockwise along the blue curve, the spin rotates by $\pi$; counterclockwise along the red curve, by $-\pi$. A quantum mechanical phase factor of $-1$ associated with that difference of $2\pi n$ leads to destructive interference of the two paths—the backscattering of electrons is suppressed in a way similar to that of photons off the antireflection coating.
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 $E_1$ and $H_1$ subbands (see the box on page 36). 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 3b. 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.

Less than one year after the theoretical prediction, a team at the University of Würzburg led by Laurens Molenkamp observed the QSH effect in HgTe quantum wells grown by molecular-beam epitaxy. The edge states provide a direct way to experimentally distinguish the QSH insulator from the trivial insulator. The two edge states of the QSH insulator act as two conducting 1D channels, which each contribute one quantum of conductance, i.e., $e^2/h$. That perfect transmission is possible because of the principle of antireflection explained earlier. In contrast, a trivial insulator phase is "really" insulating, with vanishing conductance. Such a sharp conductance difference between thin and thick quantum wells was observed experimentally, as shown in figure 3c.

**From two to three dimensions**

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 4. 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.

Liang Fu and Kane predicted that the alloy Bi$_x$Sb would be a 3D topological insulator in a special range of $x$, and with angle-resolved photoemission spectroscopy (ARPES) Zahid Hasan and coworkers at Princeton University observed the topological surface states in that system. However, the surface states and the underlying mechanism turn out to be extremely complex. In collaboration with Zhong Fang's group at the Chinese Academy of Sciences, the two of us predicted that Bi$_x$Te$_{1−x}$, Bi$_x$Se$_{1−x}$, and Sb$_x$Te$_{1−x}$, all with the layered structure in figure 4a, are 3D topological insulators, whereas a related material, Sb$_x$Se$_{1−x}$, is not.

As in HgTe, the nontrivial topology of the Bi$_x$Te$_{1−x}$ family is due to band inversion between two orbitals with opposite parity, driven by the strong spin–orbit coupling of Bi and Te. Due to such similarity, that family of 3D topological insulators can be described by a 3D version of the HgTe model (see the box). 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 4b.

Known to be excellent thermoelectric materials, Bi$_2$Te$_3$ and Bi$_2$Se$_3$ have been investigated independently, particularly at Princeton, where Hasan’s group observed in ARPES experiments the single Dirac-cone surface state of Bi$_2$Se$_3$ samples prepared by Robert Cava and coworkers. Furthermore, the group’s spin-resolved measurements showed that the electron spin indeed lies in the plane of the surface and is always perpendicular to the momentum, in agreement with theory. However, the experiments also observed bulk carriers co-existing with the topological surface states. A pure topological-insulator phase without bulk carriers was first observed in Bi$_2$Te$_3$ by Yulin Chen and Zhi-xun Shen’s group at Stanford and Bi$_2$Se$_3$ have been investigated independently, particularly at Princeton, where Hasan’s group observed in ARPES experiments on material prepared by Ian Fisher and colleagues. As shown in figure 4c, the observed surface states indeed disperse linearly, crossing at the point with zero momentum. By mapping all of momentum space, the ARPES experiments show convincingly that the surface states of Bi$_2$Te$_3$ and Bi$_2$Se$_3$ consist of a single Dirac cone. Such a state is impossible to construct in a purely 2D system. For example, a 2D graphene sheet has four Dirac cones (see the article by Andrey Geim and Allan MacDonald, PHYSICS TODAY, August 2007, page 35). The 2D HgTe quantum well at the crossover point $d = d_s$ has two Dirac cones. In a sense, the cones are spatially separated, with one placed on the top surface and the other on the bottom surface, similar to spatial decomposition illustrated in figure 1 for the 1D surfaces of a 2D system. (Particle physicists have been using similar ideas—treating a 3D lattice as the surface of a 4D lattice—in numerical simulation of fermions so as to avoid getting an unwanted doubling of neutrinos.) As we discuss below, a single Dirac cone on the surface directly leads to novel topological properties.

Topological classification of insulators

Mathematicians group geometric objects into broad topological classes. Objects with different shapes, such as a donut and a coffee cup, can be smoothly deformed into each other and can therefore be grouped into the same topological class. Mathematicians also developed the concept of a topological invariant that uniquely defines the topological class. 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 (see the article by Joseph Avron, Daniel Osadchy, and Ruedi Seiler, PHYSICS TODAY, August 2003, page 38). For a generally interacting system, the topological properties of the QH state can be described by an effective topological field theory based on the Chern–Simons theory. 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 introduced. 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. Shiuichi 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 classification. That beautiful topological band theory was soon generalized to three dimensions. The two of us and our colleagues have developed a unifying topological field theory that defines the general concept of a topological insulator in terms of a physically measurable topological field theory.

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 noninteracting 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\textsuperscript{4} can be easily integrated into electronic structure calculations to numerically evaluate the topological band invariant. However, 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,\textsuperscript{13} which can be generally defined for all insulators, with or without interactions. In the noninteracting case, both definitions agree. Surprisingly, the topological field theory can be explained in terms of elementary concepts in undergraduate-level electromagnetism.

Inside an insulator, the electric field $\mathbf{E}$ and the magnetic field $\mathbf{B}$ are both well defined. In a Lagrangian-based field theory, the insulator’s electromagnetic response can be described by the effective action $S_0 = 1/8\pi \int d^4x dt (\mathbf{E}^2 - 1/\mu \mathbf{B}^2)$, with $\epsilon$ the electric permittivity and $\mu$ the magnetic permeability, from which Maxwell’s equations can be derived. The integrand depends on geometry, though, so it is not topological. To see that dependence, one can write the action in terms of $F_{\mu\nu}$, the 4D electromagnetic field tensor: $S_0 = 1/16\pi \int d^4x dt F_{\mu\nu} F^{\mu\nu}$. The implied summation over the repeated indices $\mu$ and $\nu$ depends on the metric tensor—that is, on geometry. (Indeed, it is that dependence that leads to the gravitational lensing of light.)

There is, however, another possible term in the action of the electromagnetic field:

$$S_\theta = \frac{\theta \alpha}{4\pi^2} \int d^3x dt \mathbf{E} \cdot \mathbf{B} = \frac{\theta \alpha}{32\pi^2} \int d^3x dt \epsilon_{\mu\nu\rho\tau} F^{\mu\nu} F^{\rho\tau} = \frac{\theta}{2\pi} \frac{\alpha}{4\pi} \int d^3x dt \langle \epsilon_{\mu\nu\rho\tau} A^\mu \partial^\nu A^\rho \rangle,$$

where $\alpha = e^2/\hbar c = 1/137$ is the fine-structure constant, $\theta$ is a parameter, and $\epsilon_{\mu\nu\rho\tau}$ is the fully asymmetric 4D Levi-Civita tensor. Unlike the Maxwell action, $S_\theta$ is a topological term—it depends only on the topology of the underlying space, not on the geometry. Written using the field tensor, the term is independent of the metric.

Since the $\mathbf{E}$ field is invariant under TR, whereas the $\mathbf{B}$ field changes sign, $S_\theta$ naively breaks TR symmetry. For a periodic system, however, there are two values of $\theta$, namely $\theta = 0$ or $\theta = \pi$, that preserve the TR symmetry.\textsuperscript{12} One can easily understand that conclusion by an analogy. If we have a 1D ring with a magnetic flux inside, a general value of the flux $\Phi$ would break the TR symmetry. However, for two special values of the flux, $\Phi = 0$ or $\Phi = \hbar c/2e$, an electron’s wavefunction changes its phase by $\theta = 0$ or $\theta = \pi$ when the electron circles the ring either clockwise or counterclockwise, and TR symmetry is maintained.

If we integrate out all the microscopic fermionic degrees of freedom to obtain the effective action $S_\theta$ for all nonmagnetic insulators in the universe would fall into two distinct topological classes, described by effective topological field theories with $\theta = 0$ or with $\theta = \pi$. Unlike $\epsilon$ and $\mu$, the physically measurable $\theta$ parameter is universally quantized, with the two possible values defining the topologically trivial and nontrivial insulators, respectively—the $Z_2$ classification again.

Such classification is valid for a periodic system. For a real solid with a finite boundary, a topological insulator is insulating only in the bulk; it has an odd number of gapless Dirac cones on the surface that describe conducting surface states. If we uniformly cover the surface with a thin ferromagnetic film, an insulating gap also opens up on the boundary; the TR symmetry is preserved in the bulk but broken on the surface. The last identity of the equation above for $S_\theta$ shows that the bulk topological term is in fact a total
The field of topological insulators is growing rapidly, and many remarkable experiments have been carried out. In nonlocal transport measurements in a series of HgTe devices, the Würzburg group confirmed that transport current is carried by the QSH edge states. The topological insulators BiTeI and BiSeI fabricated in nanoribbon form at Stanford and by molecular-beam epitaxy at Tsinghua University. Scanning tunneling microscopy experiments have been carried out at Princeton, Stanford, and Tsinghua universities to probe the topological surface states. Preliminary transport measurements indicate dominant contributions from surface states.

Solving Maxwell’s equations with the topological term included leads to predictions of novel physical properties characterized by exotic excitations. The 2D QSH insulator is predicted to have fractional charge at the edge and spin–charge separation in the bulk. In introductory physics classes we learned that a point charge above a metal or an insulator can be viewed as inducing an image charge below the surface. A point charge above the surface of a 3D topological insulator is predicted to induce not only an image electric charge but also an image magnetic monopole below the surface, as shown in figure 5a. Such a composite object of electric and magnetic charges, called a dyon, would obey neither Bose nor Fermi statistics but would behave like a so-called anyon with any possible statistics. Dislocations inside a 3D topological insulator contain electronic states that behave similarly to QSH edge states.

Axioms are weakly interacting particles postulated to solve some puzzles in the standard model of particle physics (see the article by Karl van Bibber and Leslie Rosenberg, PHYSICS TODAY, August 2006, page 30). Those elusive particles are also predicted to exist inside topological magnetic insulators, systems for which the parameter above becomes dependent on position and time. Majorana fermions are distinct from the familiar Dirac fermions: They are their own antiparticles. There is still no conclusive evidence for Majorana fermions in nature. But when a superconductor is close to the surface of a topological insulator, Majorana fermions are predicted to occur inside vortices (see figure 5b). Besides teaching us about the quantum world, the exotic particles in topological insulators could find novel uses. For example, image monopoles could be used to write magnetic memory by purely electric means, and the Majorana fermions could be used for topological quantum computing.

Albert Einstein insisted that all fundamental laws of physics should be expressed in terms of geometry, and he exemplified that ancient Greek ideal by formulating the theory of gravity in terms of the geometrical curvature of space and time. Physicists are now pursuing Einstein’s dream one step further, exploring the fundamental laws expressed in terms of topological field theory. The standard model of elementary particles contains a topological term that is identical to the $S_0$ term that defines topological insulators. Even if only a small number of the predicted exotic particles are observed in topological insulators, our fundamental understanding of nature would be greatly enhanced. Such tabletop experiments could become a window into the standard model and help reveal the alluring beauty and mysteries of our universe.

**References**