

Topological insulators

This newly discovered phase of matter has become one of the hottest topics in condensed-matter physics. It is hard to understand – there is no denying it – but take a deep breath, as **Charles Kane** and **Joel Moore** are here to explain what all the fuss is about

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As anyone with a healthy fear of sticking their fingers into a plug socket will know, the behaviour of electrons in different materials varies dramatically. The first “electronic phases” of matter to be defined were the electrical conductor and insulator, and then came the semiconductor, the magnet and more exotic phases such as the superconductor. Recent work has, however, now uncovered a new electronic phase called a topological insulator. Putting the name to one side for now, the meaning of which will become clear later, what is really getting everyone excited is the behaviour of materials in this phase. Strangely, they can insulate on the inside but conduct on the outside – acting like a thick plastic cable covered with a layer of metal, except that the material is actually the same throughout. What is more, the conducting electrons arrange themselves into spin-up electrons travelling in one direction, and spin-down electrons travelling in the other; this “spin current” is a milestone in the realization of practical “spintronics”.

Topological insulators have a rather unusual history because – unlike almost every other exotic phase of matter – they were characterized theoretically before being discovered experimentally. Both of the present authors, among others, were involved in that early work, which was based on the band theory of solids – the standard quantum-mechanical framework for understanding the electronic properties of materials. We showed two things. First, special edge states (in 2D objects) or surface states (in 3D objects) allow electrons to conduct at the surface of a material that otherwise behaves as an insulator. Second, these states necessarily occur when the band structure has a certain property – a value associated with an abstract quantity called the topology (more about this later). For one of us (CK) it was an attempt to contribute to the theory of graphene – the one-atom-thick sheets of carbon

celebrated by the 2010 Nobel prize – that inspired these new ideas about topology.

But only when topological insulators were discovered experimentally in 2007 did the attention of the condensed-matter-physics community become firmly focused on this new class of materials. A related topological property known as the quantum Hall effect had already been found in 2D ribbons in the early 1980s, but the discovery of the first example of a 3D topological phase reignited that earlier interest. Given that the 3D topological insulators are fairly standard bulk semiconductors and their topological characteristics can survive to high temperatures, their novel properties could lead to some exciting applications.

How they work

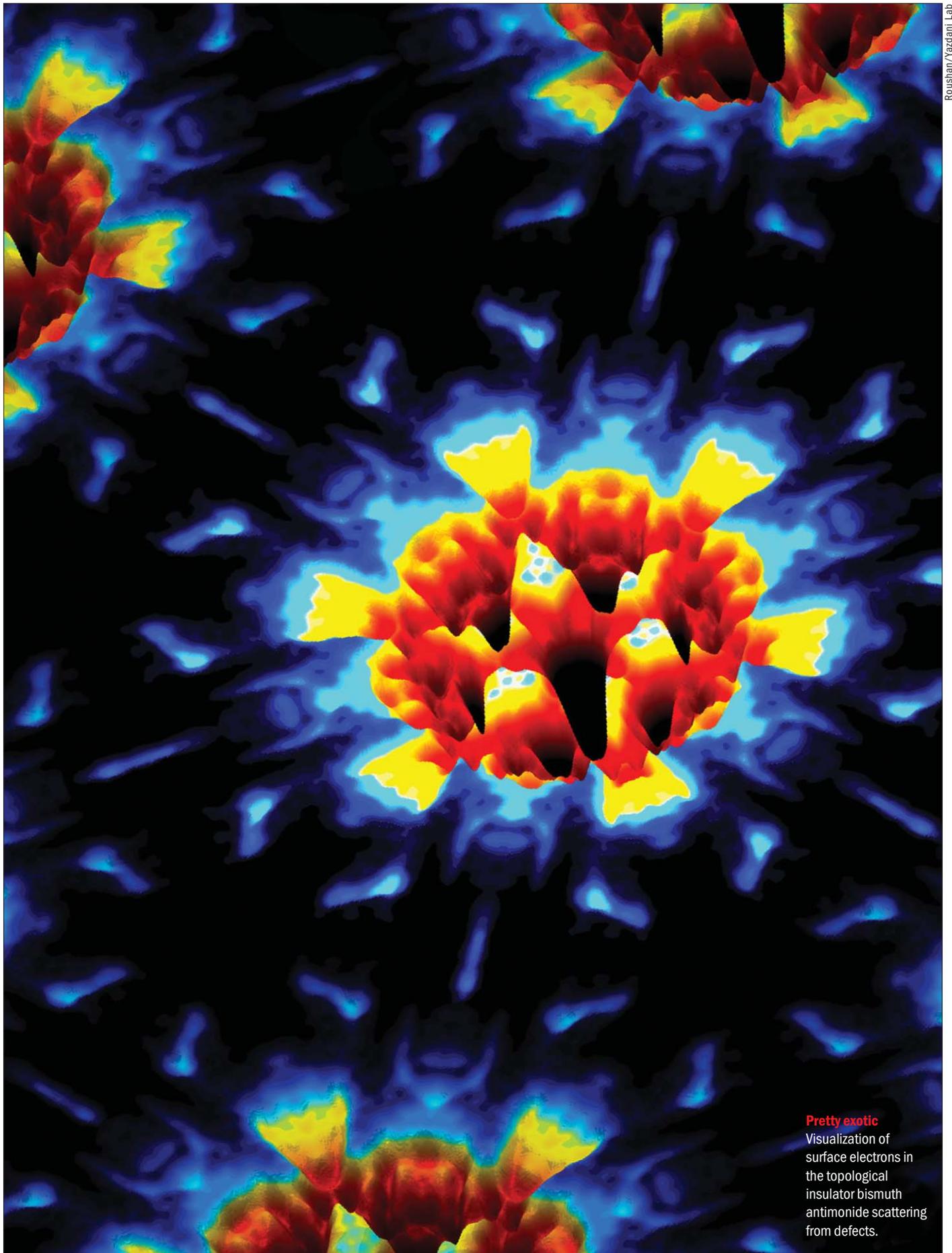
Many of the most remarkable phenomena in condensed-matter physics are consequences of the quantum-mechanical behaviour of electrons in materials. Even the insulating state (figure 1a), the most basic electronic state of matter, exhibits a conductivity that is precisely zero near a temperature of absolute zero because of a uniquely quantum-mechanical phenomenon. The insulating state occurs when an energy gap separates the occupied and empty electronic states – a behaviour that can ultimately be traced to the quantization of energy levels in an atom.

The quantum Hall state has a dramatic quantum-mechanical feature in its electrical transport. Its Hall conductance (the ratio of the electrical current to the voltage perpendicular to the current flow) is precisely quantized in units of fundamental constants when the material is near absolute zero. Topological insulators are similar to the quantum Hall state in that they exhibit “topological order”. Unlike superconductors and magnets, which have order associated with a broken symmetry, topologically ordered states are distinguished by a kind of knotting of the quantum states of the electrons. This topological order “protects” the surface states, so that they cannot be eliminated by disorder or chemical passivation, and it endows them with special properties that may be useful for applications ranging from spintronics to quantum computation.

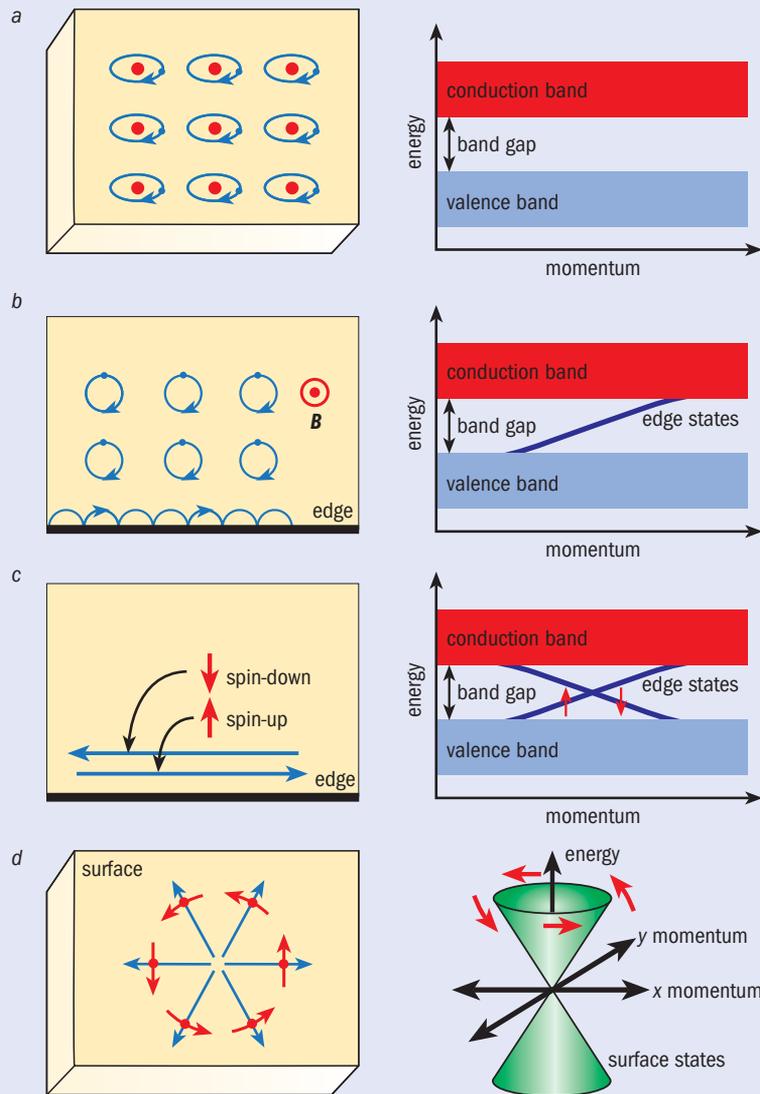
The quantum Hall state, which is the simplest topologically ordered state, occurs when electrons confined to a 2D interface between two semiconductors experience a strong magnetic field (figure 1b). The field makes the electrons experience a perpendicular Lorentz force, which causes their motion to curve into a circle, rather like the circular motion of electrons bound to an atom. And just as in an atom, quantum mechanics replaces

At a Glance: Topological insulators

- Topological insulators are insulating materials that conduct electricity on their surface via special surface electronic states
- The surface states of topological insulators are topologically protected, which means that unlike ordinary surface states they cannot be destroyed by impurities or imperfections
- Topological insulators are made possible because of two features of quantum mechanics: symmetry under the reversal of the direction of time; and the spin-orbit interaction, which occurs in heavy elements such as mercury and bismuth
- The topological insulator states in 2D and 3D materials were predicted theoretically in 2005 and 2007, prior to their experimental discovery



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.

this circular motion by orbitals that have quantized energies. This leads to an energy gap separating the occupied and empty states, just like in an ordinary insulator. At the boundary of the system, however, the electrons undergo a different kind of motion, because the circular orbits can bounce off the edge, leading to “skipping orbits”, as shown in figure 1b. In quantum theory, these skipping orbits lead to electronic states that propagate along the edge in one direction only and do not have quantized energies. Given that there is no energy gap, these states can conduct. Moreover, the one-way

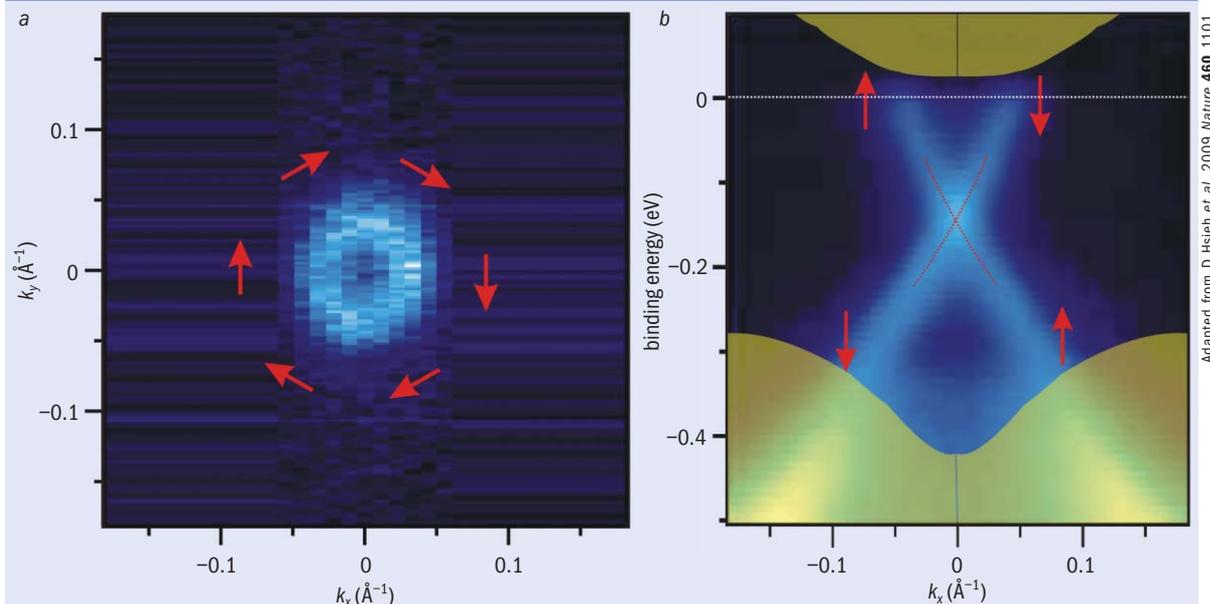
flow makes the electronic transport in the edge states perfect: normally, electrons can scatter off impurities, but given that there are no backward-moving modes, the electrons have no choice but to propagate forwards. This leads to what is known as “dissipationless” transport by the edge states – no electrons scatter and so no energy is lost as heat – and is ultimately responsible for the precise quantized transport.

Unlike the quantum Hall effect, which is only seen when a strong magnetic field is present, topological insulators occur in the absence of a magnetic field. In these materials the role of the magnetic field is played by spin–orbit coupling. This is the interaction of an electron’s intrinsic angular momentum, or spin, with the orbital motion of the electrons through space. In atoms with a high atomic number, such as mercury and bismuth, the spin–orbit force is strong because the electrons move at relativistic speeds. Electrons travelling through materials composed of such atoms therefore feel a strong spin- and momentum-dependent force that resembles a magnetic field, the direction of which changes when the spin changes.

This analogy between spin–orbit coupling and a spin-dependent magnetic field provides a way to understand the simplest 2D topological insulator – the quantum spin Hall state (figure 1c). This was first predicted in 2005, and occurs when the spin-up and spin-down electrons, which feel equal and opposite spin–orbit “magnetic fields”, are each in quantum Hall states. Like in an ordinary insulator there is thus a gap separating the occupied and empty states in the interior, but there are edge states in which the spin-up and spin-down electrons propagate in opposite directions. The Hall conductance of this state is zero because the spin-up and spin-down electrons cancel each other. The edge states can, however, conduct. They form a 1D conductor that is essentially half of an ordinary 1D conductor (a “quantum wire”, which can have spin-up and spin-down electrons moving in either direction). Like the quantum-Hall edge states, the quantum-spin-Hall edge states are protected from backscattering. However, in this case, given that there are states that propagate in both directions, the protection arises for more subtle reasons. A key role is played by time-reversal symmetry. Time reversal switches both the direction of propagation and the spin direction, interchanging the two counter-propagating modes. We will see below that time-reversal symmetry plays a fundamental role in guaranteeing the topological stability of these states.

Finally, the next tier of complication in this family of electronic phases is the 3D topological insulator. This cannot be understood using the simple picture of a spin-dependent magnetic field. Nonetheless, the surface states of a 3D topological insulator do strongly resemble the edge states of a 2D topological insulator. As in the 2D case, the direction of electron motion along the surface of a 3D topological insulator is determined by the spin direction, which now varies continuously as a function of propagation direction (figure 1d). The result is an unusual “planar metal” where the spin direction is locked to the direction of propagation. As in the 2D case, the surface states of a 3D topological insulator are like half of an ordinary 2D conductor, and are topologically protected against backscattering.

2 Topological-insulator surface states



(a) A Fermi-surface map for the surface of the topological insulator bismuth calcium selenide ($\text{Bi}_{2-x}\text{Ca}_x\text{Se}_3$) measured by spin-resolved, angle-resolved photoemission spectroscopy as a function of the surface momentum, k_x and k_y . The spin direction precesses with electron momentum around the circular Fermi surface, and opposite momenta have opposite spin. (b) The surface bands intersect at a “Dirac point” marked by the cross that is inside the bulk band gap at approximately 0.25 eV. The calcium concentration, x , is tuned so that the Fermi energy lies between the bulk valence and conduction bands.

Experimental discovery

The first key experiment in this field was the observation of the 2D quantum spin Hall effect in a quantum-well structure made by sandwiching a thin layer of mercury telluride (HgTe) between layers of mercury cadmium telluride ($\text{Hg}_x\text{Cd}_{1-x}\text{Te}$). Earlier theoretical work had predicted that, for an appropriate range of layer thicknesses, this structure should realize the 2D quantum spin Hall effect. The prediction was therefore that the structure should conduct electricity only at its edge, and also that the edge conductance at zero temperature should be $2e^2/h$, where e is the electron charge and h is Planck’s constant. Experimental results published in 2007 by a research group from the University of Würzburg, Germany, led by Laurens Molenkamp measured the electrical transport properties of such quantum-well structures and observed the predicted $2e^2/h$ conductance. It was also independent of the width of the sample, as expected for a conductance resulting only from edge states.

Measurements of electrical transport, which are ideal for probing the 2D quantum spin Hall effect, are more problematic for 3D topological insulators. The snag is that even when there is an insulating gap on the interior, there is, in practice, always a small bulk conductivity, and it is hard to separate the bulk and surface contributions to the current. A probe that couples mainly to the surface would be better and researchers therefore turned to angle-resolved photoemission spectroscopy (ARPES), which is ideally suited to the task. ARPES uses the photoelectric effect: high-energy photons are shone onto the sample and electrons are ejected. By analysing the energy, momentum and spin of these electrons, the electronic structure and spin polarization of the surface states can be directly measured.

The first 3D topological insulator to be probed in this way was the semiconducting alloy bismuth antimonide ($\text{Bi}_x\text{Sb}_{1-x}$), which had previously been predicted theoretically to be a topological insulator. In work published in 2008, a group from Princeton University led by Zahid Hasan used ARPES to map out the surface states of $\text{Bi}_x\text{Sb}_{1-x}$ and found that they had the special property (described below) characteristic of a topological insulator. Unfortunately, however, the surface states were more complicated than they had to be, prompting Hasan (and others) to search for other classes of materials that might have a simpler structure.

This search led to the discovery that bismuth selenide (Bi_2Se_3) and bismuth telluride (Bi_2Te_3) are topological insulators. These materials, which are well-known semiconductors with strong spin–orbit interactions, have a relatively large bulk energy gap (0.3 eV for Bi_2Te_3), which means that they work at room temperature. They also have the simplest possible surface-state structure (figure 2). The advantages of these materials have unleashed a worldwide experimental effort to understand their electrical and magnetic properties and to find other classes of topological insulators.

Topological phases, invariants and insulators

Two weaknesses of the simple description of topological insulators given above are that it fails to capture how robust the surface states are and how their existence is determined by the *bulk* of the material, rather than by how it was cut to make the surface. To understand the robustness and the determination by bulk properties we need to explain why these surface states are “topological” while surface states in other materials are not.

Topology is the branch of mathematics that deals with quantities that are invariant under continuous

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The advantages of topological insulators have unleashed a worldwide effort to understand their properties

Majorana fermions

One of the most exciting potential applications of topological insulators is the creation of Majorana fermions. These elusive fundamental particles have been discussed in particle physics for decades, though as yet there has been no definitive proof of their existence. Current and proposed experiments searching for a rare nuclear decay called neutrinoless double-beta decay are largely motivated by the possibility that the neutrino may be a Majorana fermion. In condensed-matter physics, Majorana fermions can occur as (non-fundamental) quasiparticles in certain special superconductors. This is allowed because a pair of quasiparticles can form a Cooper pair and disappear into the

superconductor. It is a high priority in condensed-matter physics to engineer a true Majorana fermion, in part because they could in principle be harnessed to make a fault-tolerant topological quantum computer. The race is on to come up with the best way to realize them.

The difficulty with using superconductors to make Majorana fermions is that it requires a particular kind of superconductor – called a topological superconductor – that has not yet been found. However, Majorana fermions could be made with an ordinary superconductor such as niobium if it is combined with a topological insulator. If a superconductor is placed in contact with a topological insulator, the surface

states become superconducting. Since the surface states are “half” an ordinary 2D electron system, their superconducting state is “half” an ordinary superconductor. This is precisely what is required to host Majorana fermions. There are a number of other proposals for realizing Majorana fermions with different techniques. Which one proves most feasible will depend on several practical issues. There is considerable motivation to make this happen, however, because in addition to the potential quantum-information applications, having an experimental handle on Majorana fermions would allow some of the most bizarre features of quantum mechanics to be probed.

changes. While topology can be a quite abstruse branch of mathematics, some of its concepts are familiar to anyone who has tied a knot. Consider the linked rings in the Olympic symbol, for example. Without cutting a ring it is impossible to separate them, even if the rings are bent, enlarged or shrunk. The “linking number” that formalizes this idea is an example of a topological invariant, which is a quantity that does not change under continuous changes of the rings.

Topological ideas of this type were first applied to quantum condensed-matter physics in the 1980s to understand the integer quantum Hall effect. The effect of a magnetic field in this phase, which breaks time-reversal symmetry, is to “knot” the electronic wavefunction in a non-trivial way – the wavefunctions in a quantum-Hall sample cannot be smoothly changed, with the system remaining insulating, to those of an ordinary insulator or vacuum. As a result, a metallic layer appears at the surface where the wavefunction topology changes, and the properties of this layer are not very sensitive to exactly how the surface is made.

But how can the electron wavefunctions be viewed as being knotted? Electrons in a material have wavefunctions that change as a function of the electron momentum. Changing the momentum is like moving along a piece of string in a knot, and in some materials it can be that the wavefunction evolution is so complicated that the wavefunctions cannot be continuously changed to those of an ordinary material. More specifically, the evolution of wavefunctions with momentum can be characterized by an integer, n , that is analogous to the linking number discussed above. Remarkably, there is a deep correspondence between this invariant, which comes from the interior of the sample, and the number of one-way edge modes that propagate on the boundary.

For more than 20 years it was thought that this knotting of wavefunctions required the time-reversal-breaking effect of a magnetic field and was limited to 2D quantum-well materials. In 2005 it was reported that a new kind of topological invariant (a new kind of “knotting”) was found to apply to time-reversal-invariant 2D materials and could be generated purely by spin-orbit coupling, an intrinsic property of all solids. When time-reversal symmetry is not present, this invariant no longer exists and as a result the surface state is not protected –

microscopically, the backscattering of electrons at the surface that was discussed earlier is now allowed and can cause the surface to become insulating. Further development of these ideas led to the understanding two years later that 3D materials could be in a topological phase as well, with protected surface states determined by the topology of bulk electron wavefunctions, and such materials were named “topological insulators”.

Where next?

In applied magnetic materials, spin-orbit coupling has long been studied as it determines properties such as magnetic anisotropy (that is, which directions of the magnetization are favoured) that are crucial for applications. The study of spin-orbit coupling in non-magnetic materials, in contrast, took off only recently with the advent of spintronics – electronic devices based on electron spin – and it is here that topological insulators could find their greatest potential.

The application that may be most exciting to physicists at the moment is the potential to use topological insulators to create the elusive “Majorana fermion”. Like all fermions, Majorana fermions have half-integer spin, but they are different in one regard: they are identical to their own antiparticles, which means that a pair can annihilate each other (see box above). The creation of Majorana fermions would represent a truly significant breakthrough in physics.

In the six years since the initial theoretical explorations into topological insulators, the level of interest and activity has grown exponentially. There are now dozens of experimental groups around the world, along with countless theorists, studying all aspects of these materials. With this level of activity there is great hope that some of the ambitious proposals based on topological insulators can be realized, along with others that have not yet even been conceived. ■

More about: Topological insulators

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