CONDENSED MATTER

An insulator with a twist

Experiment has now proved the existence of the predicted three-dimensional 'topological insulator' in the semiconducting alloy $Bi_{1-x}Sb_x$.

Charles L. Kane

is in the Department of Physics and Astronomy, University of Pennsylvania, 209 South 33rd Street, Philadelphia, Pennsylvania 19104-6396, USA.

e-mail: kane@physics.upenn.edu

The insulating state is the most basic electronic phase of matter. It is characterized by an energy gap for electronic excitations, which makes it electrically inert at low energies. As they report in *Nature*, Hsieh *et al.*[1] have now observed a new kind of insulator — dubbed a 'topological insulator' — that has unique conducting states bound to its surface. These surface states are unlike any other known two-dimensional electron system, and could be used to test proposed schemes for topological quantum computation.

One of the triumphs of quantum mechanics in the twentieth century was the development of the band theory of solids. An insulator has a band structure in which occupied and empty bands are separated by an energy gap. The existence of an energy gap, however, does not guarantee that a material is a simple insulator. A counterexample is the two-dimensional integer quantum Hall state, which has an energy gap due to the quantization of electronic states in a magnetic field. Despite the gap, this state is not a conventional insulator, but rather has a quantized Hall conductivity. The classification of distinct insulating band structures was pioneered in 1982 by Thouless and colleagues[2], who showed that the quantized Hall conductivity defines an integer topological invariant. This invariant is insensitive to small changes in the band structure, and can only change at a phase transition where the energy gap vanishes.

Quantum Hall states require the presence of a magnetic field, which leads to a violation of time-reversal symmetry. In the past few years, a new class of time-reversal-invariant topological insulators, which are distinguished by a different topological invariant, has been predicted for two-dimensional[3] and three-dimensional[4–6] crystals. The two-dimensional state, first predicted in graphene[7], is known as a quantum spin Hall insulator. This state was subsequently predicted[8] to exist, and was then observed[9], in $Hg_xCd_{1-x}Te$ quantum wells. In 2007, Liang Fu and I predicted that the semiconducting alloy $Bi_{1-x}Sb_x$ is a three-dimensional topological insulator[10]. In their experiment, Hsieh *et al.*[1] probed the surface of $Bi_{1-x}Sb_x$ using angle-resolved photoemission spectroscopy, and found the signature of the topological insulator state in the observed surface states.

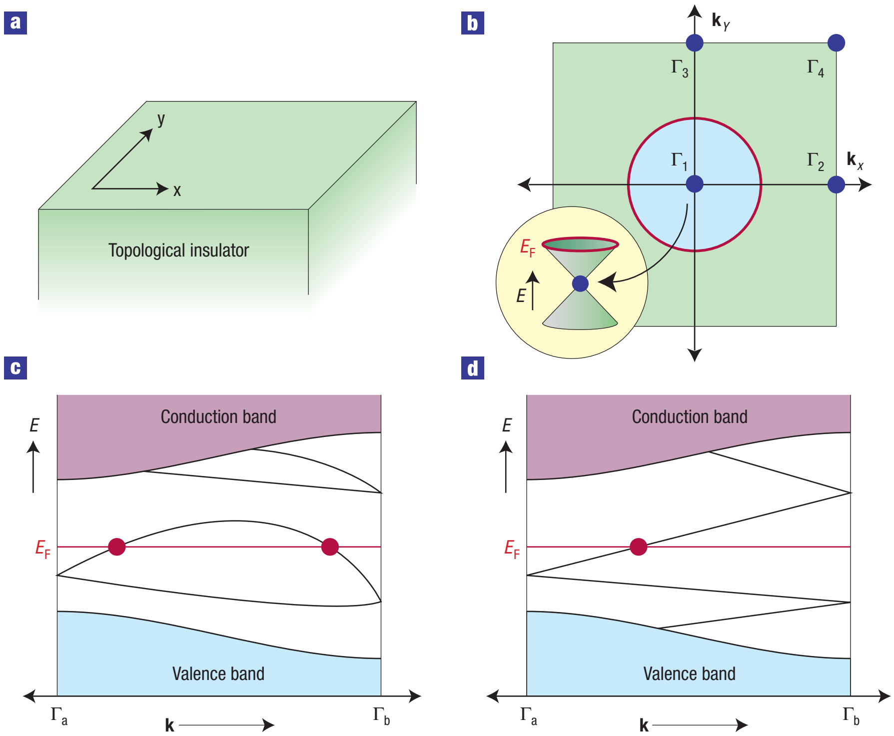

Figure 1 The surface of a topological insulator. **a**,**b**, The surface in real space (**a**) and in reciprocal space (**b**), where momentum vectors **k** in the surface Brillouin zone define Kramers degenerate points, Γ_{1-4}. **c**,**d**, Surface state dispersion between two Kramers degenerate points: in **c**, the number of surface states crossing the Fermi energy E_F is even, whereas in **d** it is odd. An odd number of crossings leads to topologically protected metallic surface states.

A distinctive property of topological insulators is the existence of gapless states on the sample boundary. Such states always occur at the spatial interface between regions that are in different topological classes. This is easiest to see by imagining a smooth limit where the band structure slowly interpolates as a function of position between the two sides. Somewhere along the way the energy gap has to vanish; otherwise the two sides would be in the same class. Gapless states are thus bound to the interface. The surface of a crystal can be viewed as an interface with the vacuum, which, like a conventional insulator, is in the trivial topological class. This guarantees the existence of gapless states on the surface (or edge) of a non-trivial insulator. These states are well known in the quantum Hall effect, which has gapless one-dimensional edge states that are unique in that they propagate in one direction only. It is impossible to have such states in an isolated one-dimensional system.

Unlike the quantum Hall effect in which the topological invariant is an integer, the invariant distinguishing a topological insulator has only two possible values. This is easiest to understand by considering the surface of a crystal (Fig 1a). Surface states can exist within the bulk energy gap, and they disperse with momentum $\mathbf{k}$ in a two-dimensional Brillouin zone. According to Kramers' theorem, time-reversal symmetry requires that all states come in degenerate pairs, at $\mathbf{k}$ and $-\mathbf{k}$. There are four special momenta, $\Gamma_{a=1-4}$, where $\mathbf{k}$ and $-\mathbf{k}$ coincide (Fig. 1b) — as well as $\mathbf{k} = 0$, the periodicity of the Brillouin zone creates three additional points.

At $\mathbf{k} = \Gamma_a$, the surface states are doubly degenerate. Between any pair $\Gamma_{a,b}$, the degeneracy is lifted by spin–orbit interactions. As shown in Fig. 1c,d, there are two distinct ways in which the states can connect. In the trivial case (Fig. 1c), it is possible to eliminate the surface states by pushing all of the bound states out of the gap. Between Γ_a and Γ_b, the bands will intersect the Fermi energy an even number of times. In contrast, in Fig. 1d the edge states cannot be eliminated. The bands will intersect the Fermi energy an odd number of times — a number that cannot be zero. Which of these alternatives occurs is determined by the topological class of the bulk band structure. In a strong topological insulator, the Fermi surface for the surface states encloses an odd number of degeneracy points. This is impossible in an ordinary two-dimensional electron system. The surface of a topological insulator defines a new two-dimensional 'topological metal' phase.

In their photoemission work, Hsieh *et al.*[1] registered an odd number of surface bands crossing the Fermi energy between two degeneracy points (as in Fig. 1d), which establishes that $Bi_{1-x}Sb_x$ is a strong topological insulator. This observation opens the door to a variety of experiments for probing the electronic and magnetic properties of this new electronic state. A particularly tantalizing prospect is that the proximity effect between an ordinary superconductor and the surface states of a topological insulator leads to a state that supports non-abelian excitations[11], which could be used for fault-tolerant quantum computation[12]. Observation of such excitations would be a first step towards realizing this goal.

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HISTORY OF QUANTUM MECHANICS

The path to agreement

Werner Heisenberg's trip to Heligoland in June 1925 is a legend. Plagued by hay fever, the 23-year old escaped to the pollen-free island in the North Sea, to return with deep insight that would change the way we think about quantum mechanics. Electrons in atoms, he came to realize, do not move in sharp orbits with definite radii and periods of rotation. As a consequence, their motion should not be described by a coordinate that depends on time, but by an array of transition amplitudes. Heisenberg, Max Born and Pascual Jordan — Paul Dirac made independent contributions — expanded the approach into what would become known as the matrix-mechanics formulation of quantum mechanics.

Only a year later, Erwin Schrödinger (pictured) presented a different formalism: wave mechanics, which uses a vastly different mathematical language — differential equations rather than the algebraic approach of matrix mechanics. Already Schrödinger was considering the relation between his own theory and the quantum mechanics of Heisenberg, Born and Jordan. In 1926, in a paper originally published in *Annalen der Physik*, he presented arguments leading to the conclusion that the two so different approaches are indeed equivalent.

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But to what degree Schrödinger proved the equivalence between the two frameworks has been the subject of some recent debate — is it actually a 'myth' that Schrödinger established the equivalence of matrix mechanics and wave mechanics, that is, that they describe the same physics? Contributing to the discussion, Slobodan Perovic argues that providing a fully fledged general proof was never the goal of Schrödinger's paper (*Studies in History and Philosophy of Modern Physics* doi: 10.1016/j.shpsb.2008.01.004; 2008).

Rather, in Perovic's view, the case has to be discussed in a specific context — the context of Niels Bohr's model of the atom. Both matrix mechanics and wave mechanics were constructed against the background of Bohr's model, and Schrödinger's main goal was, according to Perovic, to establish the coherence of the two approaches with that model. This served, not least, to underline the significance of wave mechanics. Matrix mechanics, after all, had been more successful in explaining the spectral lines of the hydrogen atom — a fact that explains, in part, why Schrödinger focused on showing explicitly (and successfully) how matrices can be constructed from eigenfunctions, whereas he only sketches rather than proves the reciprocal equivalence.

The full proof of the mathematical equivalence of matrix mechanics and wave mechanics followed only a couple of years later, notably after the Copenhagen interpretation was framed. This influential interpretation of quantum mechanics is rooted in the equivalence of the two approaches — but an equivalence, Perovic argues, in the context of Bohr's model, rather than the full proof of the isomorphism of the mathematical frameworks underlying the approaches.

Andreas Trabesinger