A topological Dirac insulator in a quantum spin Hall phase.

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Recommended with a Commentary by Bertrand I. Halperin, Harvard University.

As has been noted by various groups of authors in the recent past [1,2], there should be insulating materials whose ground states are distinguished from normal band insulators by the value of a "Z_2 quantum number" ν, which can take on one of two values, say 0 or 1, where normal band insulators have $\nu = 0$. Insulators with $\nu \neq 0$ have been termed topological insulators. The classification scheme assumes that the system has no broken time-reversal invariance, i.e., no applied magnetic field or magnetic order. Spin-orbit interaction is necessary to obtain a non-zero value of ν, but electron-electron interactions are ignored or treated as a weak perturbation.

As in ordinary insulators, topological insulators have a band structure where the Fermi level falls in an energy gap between filled and empty bands. However, a topological insulator necessarily has surface states at the Fermi level. The surface of the sample is, therefore, a reduced-dimensional metal, with some peculiar properties.

The quantum number ν is determined by the wave functions of the occupied states in the bulk band structure. It is a topological invariant, which cannot change its value, as one varies parameters in the Hamiltonian, except at a point where the energy gap vanishes between occupied and unoccupied states, or if there is a first order transition between two dissimilar ground states.

A two-dimensional system with $\nu \neq 0$ has been realized experimentally in a quantum well of HgTe, surrounded by barriers of CdTe. Its status as a topological insulator was verified by studies of the quantized electrical conductance carried by electrons at the edge of the system.[3,4] According to the theoretical picture of this system, electrons of opposite spin orientation travel only in opposite directions along an edge of the sample, and the electrical current in the experiment is carried by electrons on opposite edges with opposite spins. Two-dimensional topological insulators of this type are said to exhibit a "quantum spin Hall effect."

In principle, one could create an (anisotropic) three-dimensional material by stacking up layers of two-dimensional systems that show a quantum spin Hall state. However, there should exist a more interesting state, termed a "strong topological insulator", which is intrinsically three-dimensional, and is further removed from the two-dimensional quantum spin Hall systems. Liang Fu and C. L. Kane [2] predicted that the alloy $Bi_{1-x}Sb_x$ should be an example of this state, for an appropriate range of Sb concentration, and suggested that angle-resolved photoemission experiments (ARPES) might be the best way of detecting the predicted low-energy surface states and of confirming their peculiar properties. The ARPES experiments reported by Hsieh *et al.*, on a sample with Sb concentration $x \approx 0.1$, were intended to accomplish this goal.

A crucial step in interpreting the ARPES measurements is to carefully distinguish between contributions from surface and bulk electronic states. The assumption is that information about the momentum perpendicular to the surface is preserved when electrons are ejected from the bulk, and that measurement of the energy and the direction of the emitted electron can determine the perpendicular component k_z of the crystal momentum of the state from which the electron originated, before absorbing the photon. For bulk bands, the initial electron energy should vary with the measured k_z. For electrons ejected from surface states, however, the perpendicular momentum is not conserved, and the energy should depend only on the momentum components parallel to the surface. In order to obtain information about the k_z dispersion, and thus separate the bulk and surface bands, it is necessary to perform ARPES measurements at several different photon energies, which Hsieh *et al.* have carefully done.

What are the peculiar features of the surface bands that are hallmarks of the topological insulator state? Because the crystal structure of $Bi_{1-x}Sb_x$ has an inversion symmetry, energy levels in the bulk are doubly degenerate at each value of $\mathbf{k}$, despite the strong spin-orbit coupling. The inversion symmetry is broken at the surface, however, so that the surface states are not, in general, degenerate, except at special "Kramers degeneracy points" in the surface Brillouin zone, where $\mathbf{k}$ is equivalent to $-\mathbf{k}$, after translation by a reciprocal lattice vector. In general, there are four such points in a surface zone. For the (111) surface of $Bi_{1-x}Sb_x$, three of these occur at the $\bar{M}$ points, which are located at edge of the Brillouin zone and are equivalent to each other by the three-fold rotational symmetry of the crystal, while the fourth Kramers point occurs at $\bar{\Gamma}$, at the center of the zone. Theory predicts

that if $Bi_{1-x}Sb_x$ is a strong topological insulator, then a line from an $\bar{M}$ point to the $\bar{\Gamma}$ point should encounter surface states at the Fermi energy an odd number of times. If $Bi_{1-x}Sb_x$ were an ordinary band insulator, however, there would necessarily be an even number of these encounters. Hsieh *et al.* found five Fermi energy encounters along this line, confirming the prediction for a topological insulator.

Counting the Fermi energy encounters is not a trivial matter, as there are multiple surface bands, whose energy splittings are not always large. Indeed, two of the bands cross the Fermi energy at points along the $\bar{\Gamma} - \bar{M}$ line which are very close together. However, Hsieh *et al.* can see that there are indeed two distinct bands by observing their energy splitting at other points, where they are both below the Fermi energy but their energy splitting is larger. This is all possible because Hsieh *et al.* are using a very high-resolution ARPES measurement, with relatively low energy photons.

To further support their conclusions, Hsieh *et al.* have mapped out the Fermi surface along other directions in the surface Brillouin zone, and have shown that these are consistent with the strong-topological-insulator predictions. They have also studied bands in the *bulk* of the crystal, and shown that their behavior is consistent with the bulk structure predicted from tight-binding calculations [5], which was assumed by Fu and Kane and was an essential ingredient in their prediction that the material would be a topological insulator in the first place. A key prediction of the tight-binding band structure is the existence, at the three L points of the bulk Brillouin zone, of Dirac-like dispersions, $E_{\mathbf{k}} \approx \pm(\Delta^2 + q^2)^{1/2}$, with a small energy gap Δ, and the Fermi level inside the gap. (The quantity q is proportional to the distance between $\mathbf{k}$ and the L point, with a coefficient that depends on the direction.) The positive and negative energy states at the L points should have opposite parity, and according to Fu and Kane, the question whether or not $Bi_{1-x}Sb_x$ will be a topological insulator should depend on whether the lower energy state at the L point is symmetric, as predicted for Sb, or antisymmetric as predicted for Bi. Band structure calculations suggest that the L-point energy gap should close and open up again at a critical value $x_c \approx 0.04$, at which point the symmetries of the two states are interchanged. Hence the alloy at $x = 0.1$ should be on the Sb side, and therefore should be a topological insulator. ARPES measurements clearly confirm the Dirac-like spectrum of the bulk valence band near L, with a very small mass and a band maximum that is less than 50 meV below the Fermi energy. The measurements cannot determine the parity of the electronic states, however, so

the ARPES results for the surface bands remain crucial to the argument.

Since ARPES measurements have only a finite precision, the experiments cannot rule out absolutely the possibility that one of the observed surface bands is actually two bands that are (accidentally) close to doubly degenerate, or that there is an additional surface band that has not been detected for some other reason. The occurrence of such an undetected band would negate the argument that $Bi_{1-x}Sb_x$ is a topological insulator. However, this appears to be a very unlikely possibility. The results of Hsieh *et al.*, together with previous results and theory, should be taken as strong evidence in favor of the topological state.

References.

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