

Viewpoint

Weyl electrons kiss

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Theorists predict the possibility of topological “Fermi arc” surface states in a system with broken time-reversal symmetry.

Subject Areas: **Strongly Correlated Materials**

A Viewpoint on:

Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates

Xiangang Wan, Ari M. Turner, Ashvin Vishwanath, and Sergey Y. Savrasov

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Topology, the mathematical description of the robustness of form, appears throughout physics, and provides strong constraints on many physical systems. It has long been known that it plays a key role in understanding the exotic phenomena of the quantum Hall effect. Recently, it has been found to generate robust and interesting bulk and surface phenomena in “ordinary” band insulators described by the old Bloch theory of solids. Such “topological insulators,” insulating in the bulk and metallic on the surface, occur in the presence of strong spin-orbit coupling in certain crystals, with unbroken time-reversal symmetry [1].

It is usually believed that such topological physics is obliterated in materials where magnetic ordering breaks time-reversal symmetry. This is by far the most common fate for transition-metal compounds that manage to be insulators—so called “Mott insulators,” which owe their lack of conduction to the strong Coulomb repulsion between electrons. In an article appearing in *Physical Review B*, Xiangang Wan from Nanjing University, China, and collaborators from the University of California and the Lawrence Berkeley National Laboratory, US, show that this is not necessarily the case, and describe a remarkable electronic structure with topological aspects that is unique to such (antiferro-)magnetic materials [2]. The state they describe is remarkable in possessing interesting low-energy electron states in the bulk *and* at the surface, linked by topology. In contrast, topological insulators, like quantum Hall states, possess low-energy electronic states only at the surface.

The theory of Wan *et al.*, which uses the LDA+U numerical method, is a type of mean field theory. As such, the low-energy quasiparticle excitations are described simply by noninteracting electrons in a background electrostatic potential and, in the case of a magnetically ordered phase, by a spatially periodic exchange field. It is possible to follow the evolution of the electronic states as

a function of the U parameter, which is used to model the strength of Coulomb correlations. They apply the technique to iridium pyrochlores, $R_2\text{Ir}_2\text{O}_7$, where R is a rare earth element. These materials are known to exhibit metal-insulator transitions (see, e.g., Ref. [3]), indicating substantial correlations, and are characterized by strong spin-orbit coupling due to the heavy element Ir (iridium). In the intermediate range of U, which they suggest is relevant for these compounds, Wan *et al.* find an antiferromagnetic ground state with the band structure of a “zero-gap semimetal,” in which the conduction and valence bands “kiss” at a discrete number (24!) of momenta. The dispersion of the bands approaching each touching point is linear, reminiscent of massless Dirac fermions such as those observed in graphene.

This would be interesting in itself, but there are important differences from graphene. Because of the antiferromagnetism, time-reversal symmetry is broken, and as a consequence, despite the centrosymmetric nature of the crystals in question, the bands are nondegenerate. Thus two—and only two—states are degenerate at each touching point, unlike in graphene where there are four. In fact, the kissing bands found by Wan *et al.* are an example of *accidental degeneracy* in quantum mechanics, a subject discussed in the early days of quantum theory by von Neumann and Wigner (1929), and applied to band theory by Herring (1937). The phenomenon of level repulsion in quantum mechanics tends to prevent such band crossings. To force two levels to be degenerate, one must consider the 2×2 Hamiltonian matrix projected into this subspace: not only must the two diagonal elements be made equal, the two off-diagonal elements must be made to vanish. This requires three real parameters to be tuned to achieve degeneracy. Thus, without additional symmetry constraints, such accidental degeneracies are vanishingly improbable in one and two dimensions, but can occur as isolated points in mo-

mentum space in three dimensions (the three components of the momentum serving as tuning parameters). An accidental touching of this type is called a *diaboli- cal point*. The 2×2 matrix Schrödinger equation in the vicinity of this point is mathematically similar to a two-component Dirac-like one, known as the Weyl equation. Thus the low-energy electrons in this state behave like Weyl fermions. A property of such a diaboli- cal point is that it cannot be removed by any small perturbation, but may only disappear by annihilation with another diaboli- cal point.

Actually such diaboli- cal points were suggested previ- ously in a very similar context by Murakami [4], who argued that such a semimetallic state would naturally arise as an intermediate between a topological insulator and a normal band insulator. That theory does not di- rectly apply here, since Murakami assumed time-reversal symmetry, which is broken in Wan *et al.*'s calculations. However, inversion symmetry plays a similar role, and indeed the latter authors find that the Weyl semimetal is intermediate between an "ordinary" Mott insulator and an "axion insulator," somewhat analogous to the topologi- cal insulator. The axion insulator has a quantized mag- netoelectric response identical to that of a (strong) topologi- cal insulator, but lacks the protected surface states of the topological insulator.

What is really new and striking about the recent paper is the implications for surface states. Remarkably, they find that certain surfaces (e.g., $\langle 110 \rangle$ and $\langle 111 \rangle$ faces) have bound states at the Fermi energy, and that these states do not form the usual closed Fermi surfaces found in $2d$ or $3d$ metals. Instead, the states at the Fermi energy form open "arcs," terminating at the projection of diaboli- cal points onto the surface Brillouin zone (see Fig. 1). Fermi arcs have appeared before in physics in experi- mental studies of high-temperature cuprate superconduc- tors. However, in that context they are mysterious and puzzling, because they would seem to be prohibited by topology. The Fermi surface is by definition the bound- ary between occupied and unoccupied states, and if it terminates then one could go "around" the termination point and smoothly change from one to another, which is impossible at zero temperature. At a surface, this para- dox is avoided because the surface states may unbind into the bulk when going around the end of a Fermi arc.

This theoretical proposal provides plenty of motivation for future experiments. Observation of the Fermi arcs would be striking, and provide a useful metric to gauge the empirical ones seen in the cuprates. The bulk Weyl fermions are also interesting and would be exciting to try to observe in transport. Simple phase-space consid- erations suggest that the low-energy electrons should be remarkably resistant to scattering by impurities. Most of this theory could apply to many other materials—the only necessary conditions are significant spin-orbit cou- pling and antiferromagnetic order preserving inversion symmetry (and the latter is only essential for some of the

physics). More generally, the work widens the range of

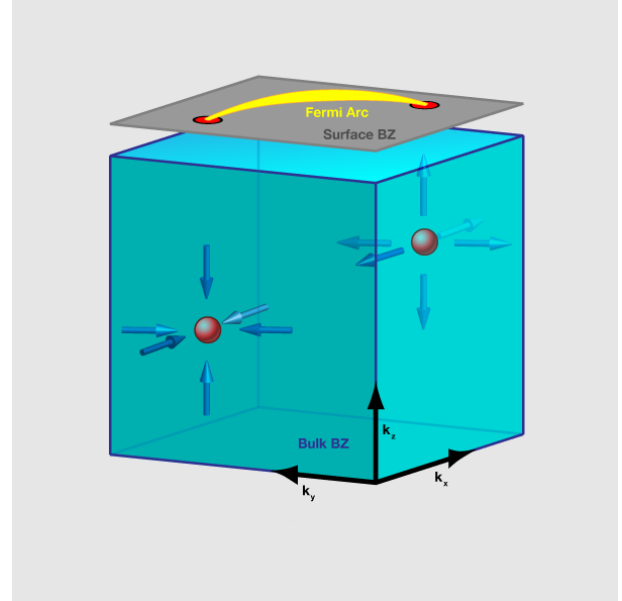


FIG. 1: Schematic image of the structure of the Weyl semimetal in momentum space. Two diaboli- cal points are shown in red, within the bulk three-dimensional Brillouin zone. The excitations near each diaboli- cal point behave like Weyl fermions. Each point is a source or sink of the flux (i.e., a monopole in momentum space) of the $U(1)$ Berry connec- tion, defined from the Bloch wave functions, as indicated by the blue arrows. The grey plane indicates the surface Brillouin zone, which is a projection of the bulk one. Wan *et al.* show that an odd number of surface Fermi arcs termi- nate at the projection of each diaboli- cal point, as drawn here in yellow. In the iridium pyrochlores studied in the paper, a nonschematic picture would be significantly more complex, as there are 24 diaboli- cal points rather than 2. (Credit: Alan Stonebraker)

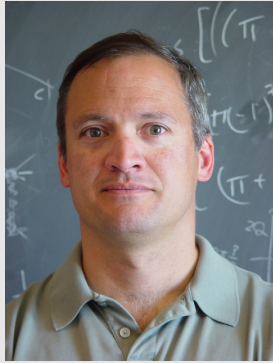
unusual states of matter that have been proposed to arise in the regime of strong spin-orbit coupling and interme- diate correlation. Despite the uncommon aspects described above, Wan *et al.*'s work is a mean-field theory, and yet more exotic possibilities have been suggested that are not describable in this way (e.g., Ref. [5]). Hopefully this is just the beginning of the theoretical and experimental exploration of this fascinating regime.

References

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