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Dawn of the TOPOLOGICAL AGE?

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Nontrivial electron band structures may enable a new generation of functional materials.

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Historians often label epochs of human history according to their material technologies—the bronze age, the iron age, and, most recently, the silicon age. From a physicist's perspective, the silicon age began with the theory, experiment, and device prototyping of a new type of material: the semiconductor. Although semiconductors had been known since the late 1800s as materials with unusual sensitivities to light, direction of current flow, and method of synthesis, not until the early 1930s did Alan Wilson make the radical proposal to describe their conduction in terms of the filling of their electronic bands.[1]

At the time, the concept of energy bands was firmly established, but electron conduction mechanisms were not clear. In the view of Felix Bloch, whose theoretical work on atomic crystals underlies the modern understanding of conduction, metals and insulators were just opposite limits of a continuous electron itinerancy. Wilson instead proposed that band filling is the control parameter: A filled valence band allows conduction only through electrons that are excited across an energy gap to another band, whereas electrons in partially filled bands can readily conduct by scattering into nearby states.

Wilson and others recognized that bandgaps were often controlled by impurities, but how impurities functioned was poorly understood. (Wilson incorrectly speculated that silicon in its purest state was a metal.) The 15 years following Wilson's proposal witnessed breakthroughs in purifying and controlling dopants in the elemental semiconductors silicon and germanium. Those advances eventually enabled the discovery of transistor action at Bell Labs in 1947. A surprise came, however, during the transistor patent preparation: The basic idea underlying the field-effect transistor had already been patented in 1930 by Julius Lilienfeld, an Austro-Hungarian physicist who had emigrated to the US in 1921.

For semiconductors, the path from theoretical understanding to device implementation was neither linear nor easily predicted. Topological materials seem to be following a similar trajectory. We have theoretical understanding and many ideas for novel devices, but ongoing materials development suggests the tantalizing possibility of our being at the dawn of a topological age. Here, we describe what it means for materials to be topological and how topology raises the prospect of revolutionary new devices.

Symmetry and invariance

Characterizing phases of matter by their symmetries is a central paradigm of physics. A magnet differs from inert iron because its internal magnetic moments consistently point in a particular direction rather than being isotropic. Similarly, a solid is different from a fluid because its atoms reside in fixed locations rather than moving freely. That prescription for understanding states of matter is usually referred to as the Landau paradigm.[2]

Over the past decade, however, awareness has grown that there is more to matter than the Landau paradigm.

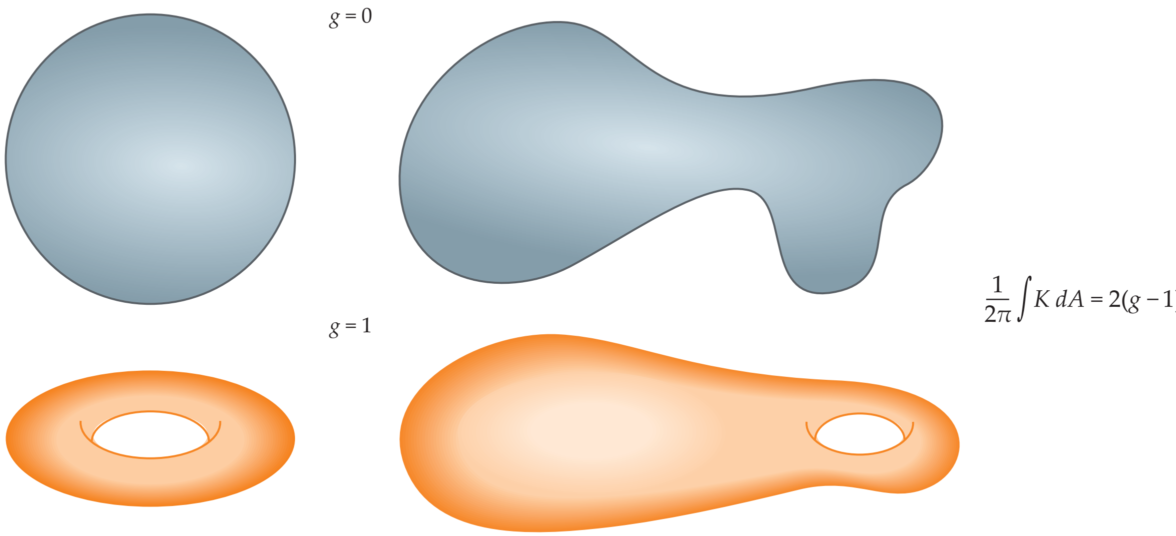

FIGURE 1. A TOPOLOGICAL INVARIANT is a property of a geometric shape that does not change when the shape is stretched or distorted. One such invariant is the genus *g*, which is given by the number of holes in the surface and is related to the integral of the Gaussian curvature *K* over the surface of the shape. Shapes with no holes in them ($g = 0$) all give the same value of this integral, as do shapes with one hole in them ($g = 1$). (Image by Donna Padian.)

Researchers are uncovering an ever-larger class of materials for which answers to basic questions, such as whether the material conducts electricity, depend not on local symmetries but on nonlocal properties called topological invariants. In much the same way that one cannot tell whether a coiled rope will form a knot when pulled tight unless one examines the full length of the rope, the electronic properties of a topological material can be determined only by examining the complete set of states in an electronic band. That nonlocality confers tremendous potential on topological materials: If a property is not defined locally, then it cannot be destabilized by local defects or fluctuations. The topological age thus promises a class of materials with unusually robust properties.

The notion of a topological invariant comes from the mathematical subfield of topology, which concerns those properties of geometric objects that are conserved under continuous deformations. The most famous such property is the genus g, an integer that counts the number of holes in a three-dimensional shape. (So $g = 0$ for a sphere, $g = 1$ for a donut, and $g = 3$ for a pretzel.) The genus is defined through the Gauss–Bonnet theorem, which states that the integral of Gaussian curvature K over the surface S of an object is quantized:

$$\frac{1}{2\pi}\int_S K\,dA = n.$$

Here n is an integer related to the genus by $n = 2(1-g)$. For example, consider a sphere with radius R. The curvature $K = 1/R^2$ is a constant, so the integral over the surface area $A = 4\pi R^2$ gives $n = 2$. That's consistent with $g = 0$, or an object with no holes in it.

The remarkable implication of the Gauss–Bonnet theorem is that if one stretches the sphere so that some parts of the surface become more curved and other parts become flatter, the integer n remains unchanged—it is topologically invariant (see figure 1). Much of the recent excitement surrounding topological electronics originates from the prospect of finding similarly invariant physical properties of electronic systems. Such a property would necessarily be robust to small perturbations or defects because integers cannot change continuously.

Topological electrons

In an isolated atom, electrons occupy discrete quantum energy levels, or orbitals. But when many atoms are arranged in a crystal lattice, the electron wavefunctions from neighboring atoms hybridize with each other and the orbitals broaden into bands of states, each having a range of energies. A state in a band describes an electron that is shared among many atoms, and the electron's wavefunction depends on the momentum $\mathbf{p}$ with which the electron hops from one atom to another. The wavefunction can be written as the product of two pieces: a plane wave that describes a free electron and a Bloch function $u_{\mathbf{p}}(\mathbf{r})$ that repeats periodically for each of the crystal's identical unit cells.[3] The Bloch function describes how the electron is affected by atomic nuclei in the unit cell, and as we will see, it contains information about the topology of the electron band.

The electron momentum $\mathbf{p}$ can have only certain restricted values. In particular, since $\mathbf{p}$ describes hopping between neighboring crystal lattice sites, the de Broglie wavelength $\lambda = 2\pi\hbar/p$ associated with the wavefunction cannot be shorter than the distance between neighboring unit cells of the crystal. The momentum in any given direction thus has a maximum possible magnitude. The space of allowable momenta is called the Brillouin zone, and its shape depends on the arrangement of atoms in the crystal.

In a discussion of an electron band's topology, the Brillouin zone plays the role of a geometric space. Closed surfaces in the Brillouin zone can be likened to geometric shapes that have an integer-valued index akin to the genus. Importantly, the Brillouin zone has effective periodic boundary conditions: Exactly opposite points on the zone's boundary are equivalent since they correspond to the same state with minimal de Broglie wavelength.

Constructing an analogue of the Gauss–Bonnet theorem for electron bands requires an analogue of curvature. As it turns out, that analogue arises from the properties of $u_{\mathbf{p}}(\mathbf{r})$. To see it, first consider the question: For a given momentum $\mathbf{p}$, where is the electron wavefunction centered in the unit cell? That question can be answered by calculating the expectation value of the position operator in the unit cell. The result is the quantity **X,** which is called the Berry connection. It can be thought of as the momentum-dependent center of the electron wavefunction in real space (see figure 2).

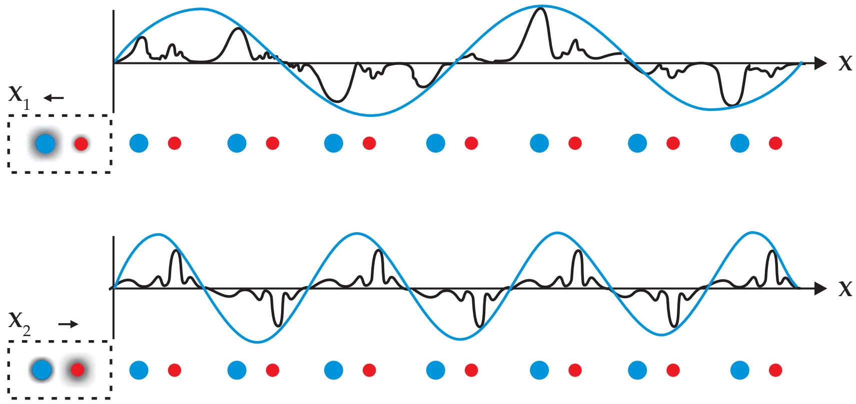

FIGURE 2. IN A CRYSTAL, AN ELECTRON STATE (black curve) is described by a slowly oscillating plane wave (blue curve) whose wavelength corresponds to the electron momentum that is modulated by a periodic Bloch function describing the electron's attraction to the atoms (red and blue circles) in the crystal's repeating unit cell. The electron probability density is shared among the atoms in the unit cell, as indicated by the shaded black areas in the outlined unit cells. The Berry connection **X**, shown above those unit cells, is a vector that can be thought of as the center of the state's density distribution. (Image by Donna Padian.)

One caveat to the analogy with the Gauss–Bonnet theorem is that **X** is not precisely defined because its definition is not gauge invariant. The Bloch functions are defined only up to an overall phase that can depend on momentum. Thus the Berry connection is like the vector potential in problems with magnetic fields in that only its curl has a physical meaning. (We will show below that the analogy with magnetic fields runs deeper.)

Imagine now the hypothetical process of accelerating and then decelerating an electron such that the electron traces a path P in momentum space before returning to its initial momentum. The electron's initial and final states are identical except for a possible overall phase factor. That phase is an example of a Berry phase (see the article by Michael Berry, PHYSICS TODAY, December 1990, page 34) and it's given by

$$\gamma_P = \frac{1}{\hbar}\int_P \mathbf{X}(\mathbf{p}) \cdot d\mathbf{p}.$$

The accumulation of a Berry phase is analogous to the phase shift a particle traversing a path in position space experiences, which is equal to the number of wavelengths in the path multiplied by 2π. Taking the same path in momentum space in the clockwise and counterclockwise directions leads to opposite signs for γ_P because it reverses the direction of momentum change $d\mathbf{p}$.

The Berry phase becomes particularly instructive if we consider how it behaves for paths in a closed two-dimensional momentum space, such as the Brillouin zone of a 2D system, which is effectively closed because opposite edges of the zone are equivalent. Consider the green path shown in figure 3, which traces the boundary of a 2D Brillouin zone. Traversing the path in the clockwise direction yields a Berry phase γ_{BZ}, whereas the counterclockwise direction gives $-\gamma_{\mathrm{BZ}}$. But opposite edges of the zone boundary describe physically equivalent states, so the clockwise and counterclockwise paths must produce equivalent changes to the wavefunction. That only happens if γ_{BZ} is either 0 or an integer multiple of 2π, leaving the wavefunction unchanged.

The condition on the Berry phase can be reformulated using Stokes's theorem to change the contour integral along the Brillouin zone boundary into a surface integral across the entire Brillouin zone. That procedure gives

$$\frac{1}{2\pi\hbar^2}\int_{\mathrm{BZ}} \Omega\, d^2p = C,$$

where Ω is the out-of-plane component of the Berry curvature, $\nabla \times \mathbf{X}$, and C is an integer known as the Chern number.

Having a nonzero Chern number requires symmetry breaking. In particular, in the Brillouin zone of a system with nonzero Chern number, the momenta $\mathbf{p}$ and $-\mathbf{p}$ are not equivalent; they have different values of **X**. That difference requires the system to break the symmetry with respect to either inversion or time reversal. The former leaves electron states unchanged when their spatial coordinates are inverted, and the latter when electron trajectories are played backwards in time. Thus, the search for topological materials has largely focused on materials that break one of those two symmetries. As we show below, only systems with broken time-reversal symmetry can have a nonzero Chern number; breaking inversion symmetry alone is insufficient. However, the coupling between electron spin and momentum may allow up and down spin species to each have a nonzero Chern number, so long as the two spin-resolved Chern numbers sum to zero.

Implications of topology

As illustrated in figure 3, a nonzero Chern number implies a winding or self-rotation in the structure of the electron wavefunction. That self-rotation is associated with the electron's physical angular momentum. For example, imagine making a wavepacket using states from a particular region of momentum space. The electron's position in the unit cell is related to the momenta of the states in the wavepacket. That relationship implies that the wavepacket's angular momentum depends on the local Berry curvature, making the Berry curvature again like a magnetic field: It's created by a broken symmetry in the material itself, and it gives electrons an orbital angular momentum.

The analogy of Berry curvature to magnetic fields becomes clearer when one considers the effects of an applied electric field **E**, which accelerates the electron. If the electron's center location **X** has a nonzero curl as a function of momentum, then as the electron accelerates, **X** shifts in the transverse direction. That shifting is known as an anomalous velocity, and it resembles the drift experienced by an electron in crossed electric and magnetic fields: Applying an electric field in a particular direction causes an electron to drift in a direction transverse to both **E** and the momentum-dependent **Ω**, which acts like a magnetic field.

One of the most striking implications of the magnetic field analogy arises from the motion of electrons at a sample's boundary. If a conductor with no intrinsic Berry curvature is subjected to a magnetic field, electrons near the boundary perform skipping orbits—they essentially roll along the boundary in a direction defined by the magnetic field. The skipping orbits persist no matter how the boundary is shaped and provide a single conducting channel for current to flow through. In a 2D electron system with a magnetic field and sufficiently high electron mobility, the skipping orbits give rise to the celebrated quantum Hall effect, with a quantized electrical conductance whose value is universal. Similarly, the self-rotation implied by a nonzero Chern number guarantees the existence of traveling edge states. Two-dimensional materials with nonzero Chern numbers have the same universal conductance, even if no magnetic field is present.

The existence of a topological invariant for electron systems subjected to a magnetic field was first identified by David Thouless, Mahito Kohmoto, Peter Nightingale, and Marcel den Nijs and bears their initials (TKNN).[4] Their topological invariant accounts for a remarkable universality of the quantum Hall effect among different samples and materials (see the article by Joseph Avron, Daniel Osadchy, and Ruedi Seiler, PHYSICS TODAY, August 2003, page 38). In fact, the TKNN invariant has allowed the universal constant $e^2/\hbar$ to be measured to more than 12 digits and now forms the basis for the metrological standard of the kilogram.[5] (See the article by Wolfgang Ketterle and Alan Jamison, PHYSICS TODAY, May 2020, page 32.) The Chern number can be thought of as a generalization of the TKNN result: Every material has a particular integer Chern number defined in the absence of any applied field. Most familiar materials have $C = 0$; recognizing the possibility of 2D materials with nonzero Chern number was a seminal insight of the topological age.

In quantum Hall systems, a magnetic field breaks time-reversal symmetry by forcing electrons to turn in spiral trajectories with a particular handedness set by the magnetic field direction. Playing those spiral trajectories backwards in time without reversing the sign of the external magnetic field produces motion inconsistent with the Lorentz force law. But edge states can exist in a topological material, even one that preserves time-reversal symmetry, if it combines broken inversion symmetry with a strong coupling between electron momentum and spin. (See the article by Xiao-Liang Qi and Shou-Cheng Zhang, PHYSICS TODAY, January 2010, page 33.) In the simplest case, those ingredients allow the two electron spin states to have nonzero but opposite Chern numbers.

To see how that situation can arise, consider that under time reversal, a left-moving spin-up electron becomes right-moving and spin-down. Thus, a topological electron band can retain time-reversal symmetry if the bands for spin-up and spin-down electrons have opposite Chern number (figure 4). The locking of edge-state directions—the two spin species moving opposite each other—is called the quantum spin Hall effect; it was discovered experimentally in 2007 following its prediction in 2003 (see PHYSICS TODAY, January 2008, page 19).

Ultimately, the locking of spin and momentum in edge states

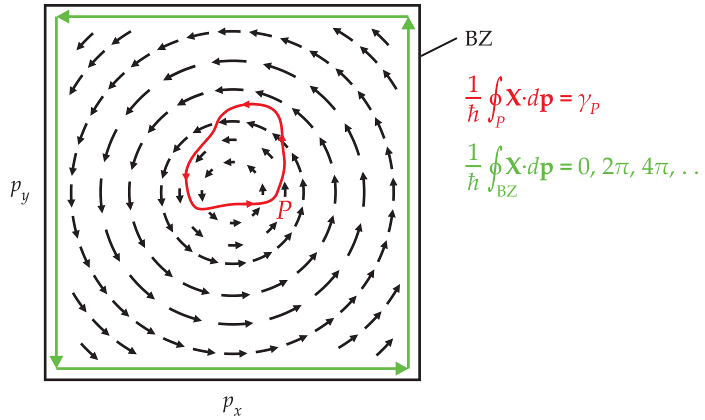

FIGURE 3. THE BRILLOUIN ZONE (BZ) is defined by the set of all possible momenta **p** for electrons in a crystal. This illustration shows the BZ for a two-dimensional crystal. The Berry connection **X** is a vector field (black arrows) in the BZ that indicates the electron wavefunction's center in the crystal's unit cell as a function of **p**. If an electron is accelerated and decelerated along some closed path P (red loop), its wavefunction acquires an overall phase γ_P whose sign depends on the direction of the path, clockwise or counterclockwise. But if that closed path runs along the BZ boundary (green loop), the phase must be a multiple of 2π. (Image by Donna Padian.)

arises from the microscopic spin–orbit coupling present in atomic orbitals. Spin–orbit coupling arises when a fast-moving electron experiences a magnetic field in its reference frame from the electrostatic potential of a nucleus. In the quantum spin Hall effect, strong spin–orbit coupling combines with broken inversion symmetry to produce a Berry curvature and a finite Chern number for each spin, even though no magnetic field is applied.

Topological bands in 3D

So far we have discussed only one example of a topological invariant: the Chern number in a 2D band that gives rise to edge states much like those in the quantum Hall effect. But 3D materials can also have electrical properties that are protected by a topological invariant. Those materials include topological insulators, which are usually narrow-bandgap semiconductors with strong spin–orbit coupling.[6] In topological insulators, an electrically insulating interior coexists with 2D metallic surface states in which electron spins are locked perpendicular to their momenta.

The 2D Chern number can also be applied to understand 3D Weyl semimetals. Such materials have special points in momentum space where their so-called topological charge is concentrated. To see why, imagine defining an arbitrary closed surface S of momentum states in the 3D Brillouin zone of some material (figure 5). Applying the same arguments about the Berry phase in 2D leads to the conclusion that the Chern number associated with the surface must be quantized. In particular,

$$\frac{1}{2\pi\hbar^2}\int_S \mathbf{\Omega}\cdot d\mathbf{A} = C_S,$$

where C_S is an integer that depends on the chosen surface S and describes a flux through the surface.

Given that C_S is an integer and cannot change continuously,

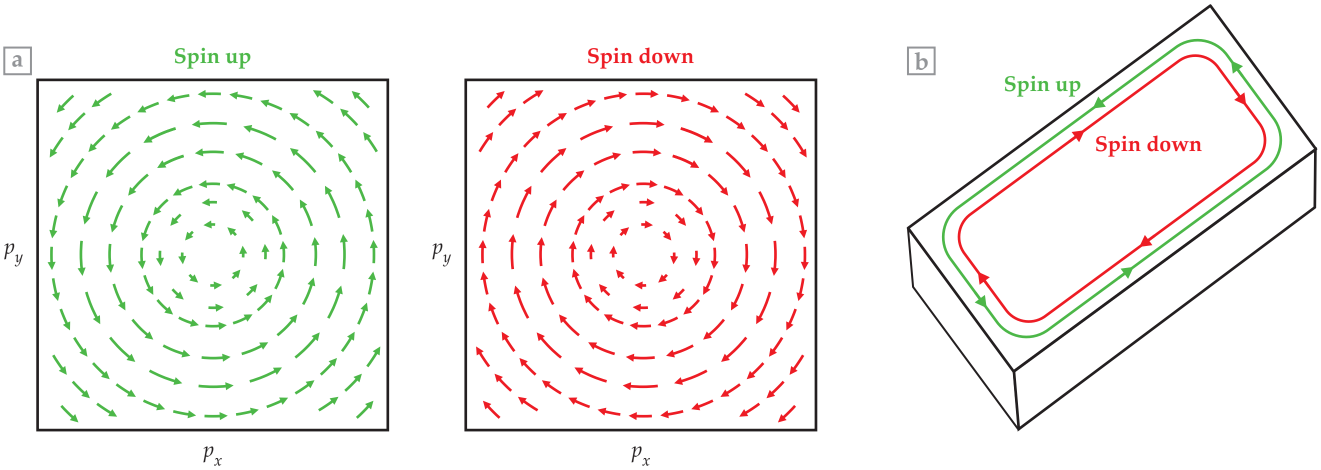

FIGURE 4. A QUANTUM SPIN HALL SYSTEM has equal and opposite Chern numbers, which describe electron wavefunction winding, for its two spin species. **(a)** The Berry connection **X**, shown here for a two-dimensional quantum spin Hall material, winds counterclockwise for up spins and clockwise for down spins, which gives Chern numbers of +1 and −1 respectively. The system remains symmetric under time reversal, which simultaneously changes **p** to −**p** and spin up to spin down. **(b)** The boundary of a quantum spin Hall material features edge states in which one spin species moves clockwise around the sample while the other moves counterclockwise. (Image by Donna Padian.)

slight distortions of the surface S cannot produce small changes to the integral. The only way for C_S to change is by a discontinuous jump, which happens when S is expanded to include a special point in momentum space known as a Weyl point. Weyl points are topological analogues to electric charges—they are monopoles of Berry flux—and the surface integral above mirrors Gauss's theorem. The points always come in pairs with opposite topological charges.

From a materials perspective, Weyl points arise when strong spin–orbit coupling causes two bands of electron states with different angular momentum to coincide in energy. The Weyl points correspond to the locations in momentum space where the two bands touch (see figure 5b) and the orbital character of the wavefunction changes abruptly. In the metals and semiconductors that make up most electronic technologies, such touching of bands is unusual. Typically, electronic bands cannot coincide in energy because of avoided crossing—the hybridization of degenerate quantum states into symmetric and antisymmetric combinations that have different energies.

In 1937, before the advent of modern topological band theory, Conyers Herring explained that two electron bands could meet—meaning they have the same energy—because of accidental degeneracies that prevent the two bands from hybridizing.[7] In that case, a perturbation that removes an accidental degeneracy can destroy the crossing and open a gap. In Weyl semimetals, however, the Weyl points are protected by the quantization of the Chern number. Only a sufficiently strong perturbation that brings two oppositely charged Weyl points together can destroy the degeneracy. Thus, Weyl semimetals are topologically protected gapless systems. Like other topological materials, they have intriguing surface states; in particular, their surfaces exhibit Fermi arcs, which are momentum states that connect the Weyl points.[8]

Identifying and classifying topological materials remains a challenge. Materials are often grouped based on their band structures; that grouping works well for semiconductors whose energy gaps largely determine functionality. But topological materials are defined not only by their energy spectra but also by the symmetries of their electron wavefunctions. Topological quantum chemistry aims to capture that complexity in order to characterize materials based on both symmetry criteria and conventional band structures.[9] The computationally intensive endeavor has unexpectedly found that an estimated 27% of all materials are topological in nature. Searches have uncovered not only new topological materials, but entirely new classes of them, such as nodal-line semimetals[10] in which two bands touch along a line rather than a point in momentum space, and higher-order 3D topological insulators[11] whose edge states exist only as lines or points along the hinges or corners of the crystal.

The interplay between topological electrons and acoustic or magnetic excitations is also a burgeoning field of study. Topological concepts can even apply to phonons and magnons themselves, which suggests a vast terrain of new materials is waiting to be explored.

Experimentally, the study of topological materials is progressing rapidly. New compounds and even whole classes of topological materials are routinely being discovered. In 2008 M. Zahid Hasan and coworkers at Princeton University first observed 3D topological insulating behavior[12] using angle-resolved photoemission spectroscopy (ARPES) in $Bi_{1-x}Sb_x$. Since then, many other topological insulators, Weyl semimetals, and nodal-line semimetals have been identified.

Technological prospects

Many materials derive their utility from their ability to either pass a current or prevent one from flowing. For example, the copper in a wire is useful because it allows electric current to flow freely, whereas the polymer encasing the wire stops the current from leaking out. Other materials pass or block heat currents, as do heat sinks on computer processors, or filter light, as do the frequency-selective lenses on protective sunglasses. From that perspective, the silicon age arose because semiconductors act as switchable valves for electrical current. We now know that pure silicon is a good insulator that only conducts if a gate voltage is applied to its surface.

New electronic materials usually have two performance

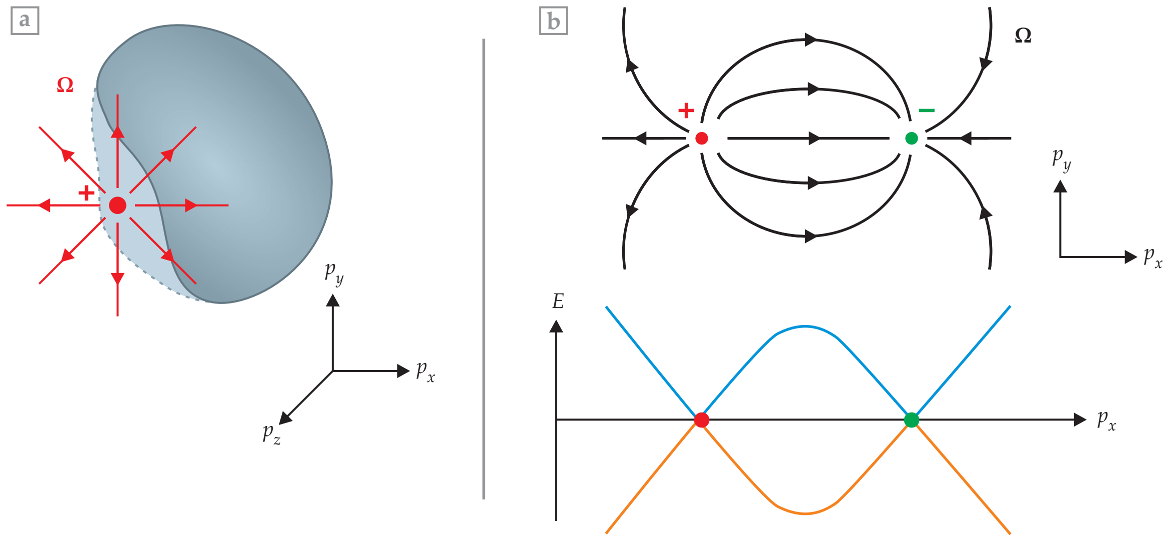

FIGURE 5. BERRY CURVATURE IN A WEYL SEMIMETAL stems from monopole sources, known as Weyl points, where two electron bands meet in momentum space. **(a)** The Berry curvature **Ω** can be depicted as a vector field (red arrows) emanating from or flowing into a Weyl point. A closed surface (gray) that does not enclose any Weyl points has Chern number $C = 0$. If that surface is expanded (dashed line) to contain a Weyl point, it abruptly attains $C = \pm 1$. **(b)** In a Weyl semimetal, Weyl points (red and green dots) come in pairs with opposite topological charge and are located at different momenta (top). At each Weyl point, two electron bands (blue and orange) meet in energy (bottom). (Image by Donna Padian.)

targets: filtering and sensitivity. The material should be able to selectively pass or block a generalized current in much the same way as silicon selectively transmits electrical current. It should also exhibit a strong response to some input, like the way silicon p–n junctions turn light into electricity. Topological materials offer the promise of truly new technologies in those areas. They are interesting filters because their Berry curvature is a kind of handedness that breaks the symmetry between clockwise and counterclockwise motion. Topological materials can therefore act like doorknobs that open when turned in the correct direction but block motion in the wrong direction.

One striking application is in spin filtering. As illustrated in figure 4, the edge states in topological insulators carry electrons with opposite spins in opposite directions. Such filtering is an essential ingredient for so-called spintronics, which aims to build electronic and computer technology based on currents of spin rather than charge.[13] The Berry curvature also implies that circularly polarized light would couple differently to the two electron species; that coupling could be used to create optical filters or logic circuits.[14]

Topological materials are unusually responsive to many kinds of applied fields because of their gapless, topologically protected electron bands. For example, the topological edge states associated with a nonzero Chern number could serve as dissipationless current-carrying channels. They have the potential to replace superconductors for some applications, and they may even function at room temperature.

More generally, the protection of low-energy states in topological materials can be exploited in ways that would give them an advantage over conventional materials in which low-energy states are often distorted by disorder. The protection of a material's electron band structure can cause its electrons to exhibit enormous mobility, which results in each electron making an outsized contribution to a current being carried.[15] Weyl semimetals are extremely sensitive to light, which may lead to a new generation of photodetectors and night-vision goggles.[16] (See PHYSICS TODAY, July 2020, page 18.) Topological semimetals also exhibit an unprecedented thermoelectric effect, the ability to convert waste heat into useful electric power.[17] Additionally, topological electrons are unusually sensitive to magnetic fields. For example, in a magnetic field the quantum levels of the electron—its Landau levels—are widely spaced in energy, and applying a magnetic field along the current direction strongly reduces the material's electrical resistance, a phenomenon known as the chiral anomaly.[18]

Whether topological materials will revolutionize our current electronic technologies remains to be seen. But ideas from topology have clearly established themselves in materials physics, and they are here to stay. They have led to predictions and observations of new materials and phenomena. Who can tell whether they will come to define our current era?

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