

## Geometrical frustration

Roderich Moessner, and Arthur P. Ramirez

Citation: *Physics Today* **59**, 2, 24 (2006);

View online: <https://doi.org/10.1063/1.2186278>

View Table of Contents: <http://physicstoday.scitation.org/toc/pto/59/2>

Published by the *American Institute of Physics*

---

### Articles you may be interested in

#### [Frustration by design](#)

*Physics Today* **69**, 54 (2016); 10.1063/PT.3.3237

#### [Do quantum spin liquids exist?](#)

*Physics Today* **69**, 30 (2016); 10.1063/PT.3.3266

#### [Frustration in physics](#)

*Physics Today* **35**, 78 (2008); 10.1063/1.2915237

#### [New candidate emerges for a quantum spin liquid](#)

*Physics Today* **60**, 16 (2007); 10.1063/1.2711623

#### [Quantum criticality](#)

*Physics Today* **64**, 29 (2011); 10.1063/1.3554314

#### [The quantum spin Hall effect and topological insulators](#)

*Physics Today* **63**, 33 (2009); 10.1063/1.3293411

---

## The *Physics Today* Buyer's Guide

The latest tools,  
equipment and  
services you need.  
**Fast track your  
search today!**



PHYSICS  
TODAY

Shop with a more powerful search engine now.

# Geometrical Frustration

**When interactions between magnetic degrees of freedom in a lattice are incompatible with the underlying crystal geometry, exotic phenomena such as spin ice and spin liquid phases can emerge.**

Roderich Moessner and Arthur P. Ramirez

The ancient Greeks were aware of the phenomenon of magnetic order in lodestone, a type of rock containing the ferromagnet magnetite  $\text{Fe}_3\text{O}_4$ . Magnetic moments in a ferromagnet tend to align and thereby sum to an easily observed macroscopic magnetic moment. The absence of such a moment even in ordered antiferromagnets is the reason their discovery is comparatively recent. It had to await the development of Louis Néel's microscopic theory of spin interactions in the 1930s and the neutron diffraction measurement of  $\text{MnO}$  in 1949 by Clifford Shull and Stuart Smart.

There are magnets, however, that today present greater experimental and theoretical challenges than those posed by simple antiferromagnets in the 1930s.<sup>1</sup> The origin of their complex and varied behavior is remarkably simple and can be illustrated by as few as three spins on a triangular lattice. Once two of the spins on an elementary triangle are antialigned to satisfy their antiferromagnetic interaction, the third one can no longer point in a direction opposite to both other spins (see figure 1). Thus, not all interactions can be minimized simultaneously—that is, exist in their lowest energy state. In other words, antiferromagnetic interactions are incompatible with triangular lattice symmetry, a situation known as geometrical frustration.

The antiferromagnetic triangle is the simplest case in which a conflict arises between the geometry of the space inhabited by a set of degrees of freedom and the local correlations favored by their interactions. This phenomenon is one aspect of a powerful paradigm for discovery over the past few decades—namely, our ability to experimentally manipulate the space in which magnetic, charge, or vibrational degrees of freedom interact. Two other particularly well-studied aspects are low effective dimensionality for electronic systems and tunable optical lattices for systems of cold atoms.

The study of geometrically frustrated magnets is concerned with what happens when lattice geometry inhibits the formation of a simple, ordered, low-temperature spin configuration. Typically, geometrical frustration gives rise

to a degenerate manifold of ground states rather than a single stable ground-state configuration, leading to magnetic analogues of liquids and ice. Not surprisingly, even slight perturbations induce instabilities in such systems and prompt the emergence of further unusual phenomena, even including an incarnation of artificial

electrodynamics in which the frustrated magnet acts as an “ether” for novel magnetic excitations.

Frustrated magnets thus lie at the crossroads of two fundamental enterprises in condensed matter physics. On the applied side, the instabilities exhibited by frustrated magnets open a window on the richness of nature realized in different materials. On the fundamental side is the search for principles that help organize the variety of behavior we observe around us. This article addresses two possible principles: Underconstraint, which here arises for spins residing on a weakly connected lattice whose geometry frustrates their mutual interactions, and emergence, the dynamical generation of new types of degrees of freedom.

## Frustration leads to degeneracy

To understand the central features of frustrated magnetism, consider a simple set of model Hamiltonians that account only for antiferromagnetic interactions between nearest neighbors:

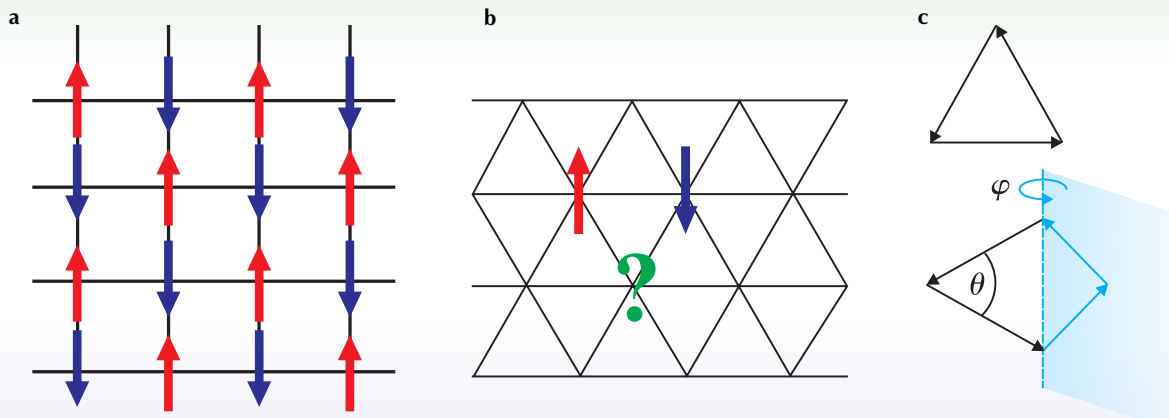
$$H = J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j.$$

In this equation, a positive exchange energy  $J$  favors antiparallel alignment of the spins  $\mathbf{S}$ , labeled by their site indices  $i$  and  $j$ , and the sum is taken over nearest-neighbor bonds. For the moment, we restrict our attention to the case where the spins are classical, either as discrete Ising-model spins ( $S = \pm 1$ ) or continuous, three-component Heisenberg vector spins  $\mathbf{S} = (S_x, S_y, S_z)$  of fixed spin length  $|\mathbf{S}|$ .

The hallmark of frustration in such models is a large ground-state degeneracy. For continuous spins, a simple counting argument can give the size of the degeneracy: The number of degrees of freedom in the ground state,  $F$ , is estimated to be  $D - K$ , where  $D$  is the total number of degrees of freedom of the spins and  $K$  the number of constraints that must be satisfied to put the system into a ground state.

The idea essentially comes from linear algebra, in which a system of  $K$  equations for  $D$  variables is expected to have a solution space of dimension  $F = D - K$ . Here, as there, the expectation may be wrong because the constraints imposed by the equations may not be independent (like  $2x = 4$  and  $4x = 8$ , for example), or because they may be mutually exclusive (like  $2x = 4$  and  $4x = 7$ ).

*Roderich Moessner is a research scientist at CNRS and the École Normale Supérieure in Paris. Art Ramirez is director of the device physics research department at Lucent Technologies' Bell Labs.*



**Figure 1. A geometrically frustrated system** is one in which the geometry of the lattice precludes the simultaneous minimization of all interactions. **(a)** In the unfrustrated antiferromagnet on the square lattice, each spin can be antialigned with all its neighbors. **(b)** On a triangular lattice, such a configuration is impossible: Three neighboring spins cannot be pairwise antialigned, and the system is frustrated. **(c)** The ground states of a cluster of Heisenberg spins have zero total spin, so the vector sum of an elementary group of spins must add up to zero. A cluster of three spins forms a unique structure, whereas four spins form a family of degenerate ground states, with  $\theta$  and  $\phi$  the structure's two degrees of freedom.

James Clerk Maxwell introduced such counting in the context of elastic systems in 1864, and John Chalker of Oxford University and one of us (Moessner) applied it to frustrated spin systems in 1998. It can be illustrated most simply in clusters of  $q$  mutually interconnected spins, for which the above Hamiltonian can be rewritten as

$$H = \frac{J}{2} \left( \sum_{i=1}^q \mathbf{S}_i \right)^2.$$

Each three-component Heisenberg spin has two degrees of freedom. With its length fixed, each spin is free to take any value on the surface of a sphere, with the two degrees of freedom parameterized, for instance, by latitude and longitude. Obviously, all states in which the total spin sums to zero are ground states, provided such states exist. This condition supplies three ground-state constraints, one for each component of the total spin. Hence, there are  $D - K = 2q - 3$  degrees of freedom left. Three of those correspond to global rotations, but the remaining  $2q - 6$  are genuine unconstrained degrees of freedom, even in the ground state.

The symmetric arrangement of three mutually interconnected spins ( $q = 3$ ) takes the form of a triangle in spin space, for which there are no internal degrees of freedom; one thus finds a unique  $120^\circ$  ground-state spin structure. In contrast, a cluster with four interconnected spins ( $q = 4$ ), arranged symmetrically on the corners of a tetrahedron, is underconstrained: The degenerate ground state has two internal degrees of freedom, parameterized by angles  $\theta$  and  $\phi$  as shown in figure 1c.

Maxwellian counting can be generalized to treat lattices rather than just isolated clusters of spins. To maximize the ground-state degeneracy for a fixed number of spins, one must minimize the number of constraints. Lattices that are made up of vertex-sharing clusters do just that. In the two-dimensional kagome lattice, for example, each site belongs to only two triangles (see figure 2); in the less-frustrated triangular lattice, each site belongs to six (see figure 1).

By this counting method, the most degenerate—and thus most frustrated—lattice readily realizable in three dimensions or less is the one made up of vertex-sharing

tetrahedra, the pyrochlore lattice pictured in figure 2b. Indeed, the number of degrees of freedom in the pyrochlore ground state is an extensive property: It equals the number of tetrahedra!

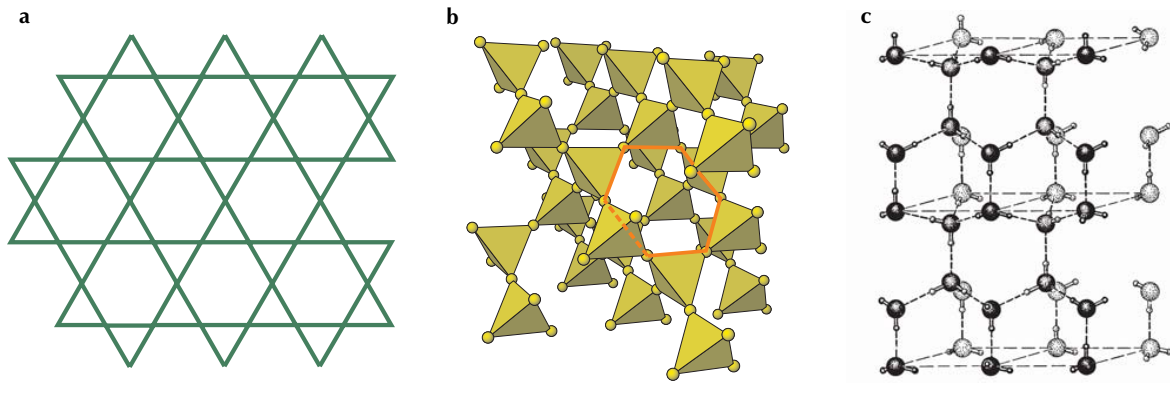
The huge ground-state degeneracy is accidental in that two different ground states are not generally related by any symmetry operation. Normally, fine-tuning some parameters is required to produce such an accidental degeneracy. However, in the pyrochlore lattice, the symmetry of the tetrahedron takes care of that fine-tuning by ensuring that the interactions have equal strength; that is, the symmetry allows a choice between which bonds to frustrate.

### Spin ice and water ice

For materials with Ising spins, geometrical frustration takes a different form. An Ising spin has only two discrete orientations—up or down—because it is constrained to point along one axis. Unlike in the continuous case, the spin cannot exhibit small deviations from those directions. Consequently, its number  $W$  of ground states is countable and can be used to define a residual entropy  $S_0$  via Boltzmann's relation  $S_0/k_B = \ln W$ .

An approach analogous to Maxwellian counting for continuous spins adapts an estimate of the entropy made by Linus Pauling for water ice.<sup>2</sup> Pauling's description of the low-temperature ordering of protons in crystalline ice was perhaps the first recognition of the significance of geometrical frustration. The proton ordering in ice turns out to be locally equivalent to the physics of a frustrated pyrochlore Ising magnet as first noted by Philip Anderson of Princeton University.<sup>3</sup> Again, to estimate  $W$  one separately evaluates the total number of states on the one hand and the action of the constraints on the other.

For example,  $2^N$  possible states exist on the pyrochlore lattice—each of its  $N$  Ising spins points either up or down. As for the constraints, out of the  $2^4$  possible spin states on a tetrahedron, only six (a fraction of  $\frac{3}{8}$ ) are actually ground states, namely, those in which two spins point up and two down, so that their sum equals zero. Pauling's estimate amounts to treating the constraints imposed by different tetrahedra as if they were independent; that is only an approximation, but turns out to be a rather good one.



**Figure 2. Frustrated lattices.** (a) The kagome lattice consists of vertex-sharing triangles. (b) The pyrochlore lattice is a network of vertex-sharing tetrahedra. The orange hexagonal loop is discussed in figure 4. (c) Hexagonal ice consists of protons (small spheres) that reside on the bonds between two oxygen atoms (large spheres). The positions of the oxygens are uniquely determined, but there are exponentially many allowed proton configurations. (Figure 2c is adapted from ref. 2.)

Because the number of tetrahedra equals  $N/2$ , Pauling's estimate for the number of ground states is thus  $W = (3/8)^{N/2} 2^N$ . That implies an entropy per spin of  $S_0/k_B N = (1/N) \ln W = \frac{1}{2} \ln \frac{3}{2}$ .

How can one observe this ground-state degeneracy and the resulting entropy  $S_0$ ? As the high-temperature entropy equals that of free spins,  $S_f = Nk_B \ln 2$ , it suffices to measure the amount of entropy  $\Delta S$  that leaves the system as it cools to temperatures at which only the ground states are accessible. At those temperatures,  $S_0 = S_f - \Delta S$ .

This residual entropy can be demonstrated explicitly in the case of spin ice, a frustrated ferromagnet whose spin states at low temperature mimic the configurations of the hydrogen ions in water ice.<sup>3</sup> Mark Harris of Rutherford Appleton Laboratory and Steve Bramwell of University College London discovered spin ice in 1997 and realized that holmium titanate ( $\text{Ho}_2\text{Ti}_2\text{O}_7$ ) can be understood as a frustrated Ising magnet on the pyrochlore lattice.<sup>4</sup>

In common water ice the location of oxygen atoms is strictly periodic, as pictured in figure 2c, whereas the location of the hydrogen ions is not. At atmospheric pressure, ice forms a hexagonal structure that preserves the H–O distance found in water molecules. That distance, however, is far less than half the distance between oxygen atoms. Therefore, each hydrogen atom can occupy one of two sites: close to or far from a particular oxygen atom. One “ice rule” states that around each oxygen atom are two hydrogens that are close by, as in an  $\text{H}_2\text{O}$  molecule, and two that are far away. Because only 6 (of the 16 possible) configurations achieve that arrangement, one obtains the Pauling estimate for the entropy per hydrogen as derived above,  $S_0/k_B N = \frac{1}{2} \ln \frac{3}{2}$ .

The approximate equivalence of pyrochlore spin ice to water ice follows from identifying the centers of the pyrochlore tetrahedra with the location of the oxygen atoms. The spins are then located at the midpoint of the bond between a pair of neighboring oxygens. The axes for the Ising spins are precisely those bond directions, and each spin points in the direction of the oxygen atom closest to the proton along that bond. The ground-state entropy of pyrochlore spin ice is thus expected to be approximately the same as it is in water ice.

One of us (Ramirez) and coworkers tested that expect-

ation<sup>5</sup> by measuring the specific heat of dysprosium titanate  $\text{Dy}_2\text{Ti}_2\text{O}_7$ , an Ising pyrochlore similar to  $\text{Ho}_2\text{Ti}_2\text{O}_7$ . Indeed, the resulting entropy agreed with the theoretical Pauling value for ice to within a few percent (see figure 3). In the absence of any structural disorder in the host compound, a nonzero entropy indicates that spin ice represents a new state of magnetism.

### Local zero-energy modes

The residual entropy is due to the existence of a large number of ground states. How can the system fluctuate between them? One extreme possibility occurs in a ferromagnet, where all spins point in the same direction in a ground state. To get to a different ground state, all spins of the system would need to flip and be reoriented together. The other extreme occurs in a completely noninteracting paramagnet, where each spin can be separately flipped, because the energy does not depend on its orientation.

A frustrated magnet, even at zero temperature, can be closer to the paramagnet: A local rearrangement of a finite cluster of spins is possible at zero cost in energy while still preserving the ground-state constraint that the sum of all the spins in a cluster add up to zero.<sup>6</sup> As shown in figure 4, the pyrochlore lattice bears this out. The smallest such cluster is a group of spins (marked by green crosses) arranged in a hexagon. Reorienting a single spin by  $\delta\mathbf{S}$ , say, would change the total spin of the two tetrahedra it belongs to by  $\delta\mathbf{S}$ . However, changing the value of neighboring spins in the cluster by equal and opposite amounts  $\pm\delta\mathbf{S}$  ensures that the sum of those changes vanishes for each individual tetrahedron.

In 2002 Oleg Tchernyshyov of Johns Hopkins University, Shivaji Sondhi of Princeton University, and one of us (Moessner) considered a model in which spin rearrangements around such hexagons are dominant. The resulting spin correlations agree very well with measurements of Seung-Hun Lee of the University of Virginia, Collin Broholm of Johns Hopkins, and coworkers on the spinel compound zinc chromium oxide ( $\text{ZnCr}_2\text{O}_4$ ), in which the chromium ions, Heisenberg spins with  $S = \frac{3}{2}$ , form a pyrochlore structure. The work confirmed the existence of hexagonal modes in this compound.<sup>7</sup>

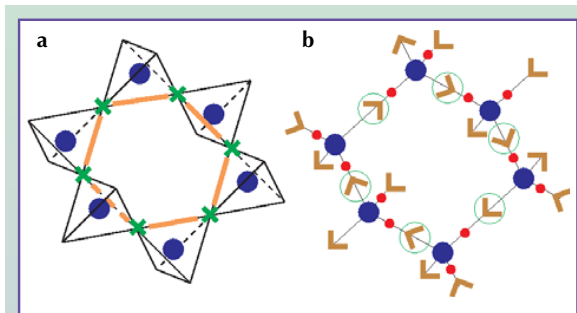
### Algebraic correlations without criticality

The nature of correlations is fundamentally influenced by conservation laws, and in a class of geometrically frustrated magnets this connection has an interesting consequence. One might naively expect that reorienting local spins in a cluster would destroy long-range order, as it does in a paramagnet. That expectation, however, would be quite wrong. Rather, the ground-state constraint implies a local conservation law that leads to a theory formally equivalent to conventional magnetostatics.<sup>8</sup>

In the simplest case of the spin-ice model, the orientation of the magnetic moments defines a divergence-free (though artificial) magnetic flux  $\mathbf{B}$  on the links of the ice lattice as shown in figure 4b, where the spins are denoted by arrows. The ice rules dictate that two spins point toward each oxygen atom and two point away. As in Kirchhoff's law for current flow in electrical circuits, the total amount of flux that enters or leaves each node, or oxygen atom, is zero. Consequently, the magnetic flux, like the electrical current, is conserved and therefore has zero divergence:  $\nabla \cdot \mathbf{B} = 0$ .

The conservation law has important implications: Correlations between spins are enhanced because fluctuations that do not respect the zero-divergence constraint are prohibited. In fact, the simplest hydrodynamical theories of correlations have as their starting point the idea that correlations at long times and distances are fundamentally governed by underlying conservation laws.

A detailed analysis of the spin correlations in the presence of the constraint  $\nabla \cdot \mathbf{B} = 0$  leads to a theory of precisely the same form as magnetostatics, in which the absence of magnetic monopoles is, of course, also a vital ingredient. The statistical correlations between different spins therefore follow a dipolar form like  $(3\cos^2\theta - 1)/|\mathbf{r}|^3$ . That is, the correlations decay like a power law with dis-



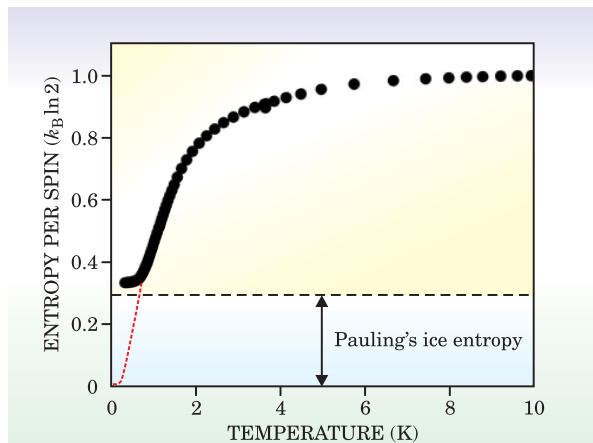
**Figure 4. Local modes.** (a) A hexagonal loop (orange), consisting of edges of a group of tetrahedra in the pyrochlore lattice of figure 2b, can support a zero-energy mode. The mode involves reorienting neighboring spins (green crosses) by equal and opposite amounts  $\delta S$ . The rearrangement preserves the ground-state constraint for each tetrahedron—the sum of the spins remains zero. (b) Ice representation of such a loop. Oxygen atoms (blue) reside in the centers of the tetrahedra, while the spins (brown) sit on the midpoints of the bonds and point in the direction of the hydrogen atoms (red). Inverting the six encircled spins pointing clockwise around the loop produces another energetically equivalent ground state.

tance and exhibit a nontrivial angular dependence. Here,  $\mathbf{r}$  is the distance vector between the spins and  $\theta$  the angle between  $\mathbf{r}$  and the axis along which the spins are constrained to point. In Fourier space, the correlations show up as a characteristic bow-tie motif with a pinch point at its center (see figure 5). Martin Zinkin of Oxford University first noticed such bow ties in frustrated magnetism in 1996.

Crucially, the dipolar correlations between spins are algebraic but not critical. The adjectives “algebraic” and “critical” are normally used interchangeably in condensed matter physics because the critical point—between paramagnetic (disordered) and Néel (ordered) phases, say, in an unfrustrated antiferromagnet—typically gives rise to correlations that decay algebraically. But the frustrated magnet is unusual; it exhibits algebraic correlations between spins but does not sit at a point sandwiched between a disordered and an ordered phase. Rather, the ground-state constraint is strong enough to prevent an exponential decay of correlations, but too weak to induce long-range order. Similarly, and somewhat reassuringly, the algebraic decay of a dipole's real magnetic field at long distances does *not* indicate that electromagnetism sits at a critical point, delicately balanced between an ordered and a disordered phase.

### Artificial light

What are the effects of adding quantum fluctuations to a frustrated system? Those fluctuations can be added in the framework provided by a class of models introduced in 1988 by Daniel Rokhsar of University of California, Berkeley, and Steve Kivelson of Stanford University in the context of high-temperature superconductors.<sup>9</sup> The models include the simplest possible quantum dynamics consistent with the classical ground-state constraint. Because the spins cannot fluctuate individually but only as loops, one must add a perturbation to the simple exchange Hamiltonian so that loops of six spins (as pictured in figure 4) are allowed to tunnel between one classical ground state



**Figure 3. The entropy  $S$**  of the spin-ice compound dysprosium titanate  $\text{Dy}_2\text{Ti}_2\text{O}_7$ , as a function of temperature  $T$ . At high  $T$ ,  $S = k_B \ln 2$  per spin, the same as for free spins. Cooling the system causes the entropy to drop as correlations develop between spins. An unfrustrated magnet follows the plot's schematic red line down to zero entropy because the system assumes a unique ground state. In spin ice, geometrical frustration creates an exponentially large number of degenerate ground states. The large degeneracy manifests itself in a non-vanishing entropy, which is close to the value that Linus Pauling predicted for ordinary water ice. (Adapted from ref. 5.)

in which the arrows point clockwise and another in which they reverse direction. Analysis of the Rokhsar–Kivelson model that corresponds to this type of system reveals a phase described by an effective Maxwell Hamiltonian:  $H = \mathbf{E}^2 + c^2\mathbf{B}^2$ , where  $\mathbf{E}$  is related to  $\mathbf{B}$  in the same way that the electric field is related to the magnetic field in standard electromagnetism.<sup>8</sup>

The formal equivalence to the Maxwell Hamiltonian immediately implies the presence of artificial photons in the frustrated system, traveling at the speed of artificial light,  $c$ . And this speed can be tuned by changing microscopic parameters of the underlying model. A tunable speed of light is nothing unusual in itself, of course; the speed of ordinary light can, after all, be reduced inside a dielectric.

The frustrated magnet is, however, fundamentally different from a dielectric. Take away the dielectric and one is still left with electromagnetic waves in vacuo. Take away the frustrated magnet and the artificial electromagnetism is lost altogether. The frustrated magnet thus acts as an “ether” to the artificial light.

The artificial photon is really a complex coherent superposition of spin degrees of freedom. Spins, in turn, are not fundamental particles at all, but rather a low-energy description of some degrees of freedom of a solid. A little high-energy physicist living inside our frustrated system would be in for quite a surprise upon discovering the degrees of freedom of the solid during a scattering experiment between artificial photons.

From that perspective, as MIT’s Xiao-Gang Wen has emphasized, it is not inconceivable that particles we normally think of as elementary are, in fact, emergent composite objects in a universe that, at high energies, looks increasingly messy rather than increasingly simple. The phenomenon of one set of degrees of freedom (like spins) giving rise to a qualitatively different set (like photons) is known as emergence. This ability of condensed matter systems to mimic spontaneously and collectively different ones—possibly unknown or otherwise unrealizable—is among their most fascinating properties.

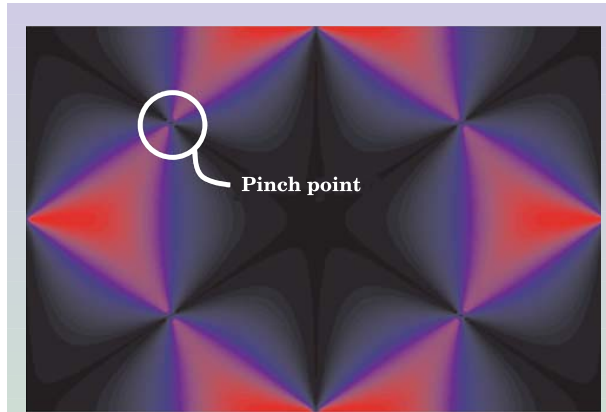
### Cooling to observe frustration

No experimental system is yet known that provides us—at least unequivocally—with the coherent quantum dynamics just discussed. The collective quantum dynamics within clusters of spins is rather fragile, and other perturbations to the model Hamiltonian generally become important before the quantum fluctuations do. What happens in different temperature regimes?

**The spin-liquid regime.** At high temperatures, no spin correlations are present, and any magnet is a simple paramagnet. When the magnet is cooled, the spins start to form into clusters that obey the ground-state constraint.

That evolution happens on a temperature scale determined by the exchange energy  $J$ , or more precisely the Curie–Weiss temperature  $\theta_{\text{CW}} = zJS(S + 1)/3k_{\text{B}}$ , which is the product of  $J$  with the number of nearest neighbors  $z$  and the spin length  $S(S + 1)$ . The temperature regime below  $\theta_{\text{CW}}$  is known as the spin-liquid regime because, as in an ordinary liquid, the interactions are strong but there is no long-range order. Such spin liquids can nevertheless, as we’ve seen, exhibit subtle correlations in the absence of long-range order.

**The nonperturbative low-temperature regime.** For the idealized frustrated Hamiltonian, a spin-liquid or spin-ice regime can exist all the way down to zero temperature. One might worry that an exponential ground-state degeneracy and the resulting residual entropy are inconsistent with the third law of thermodynamics, which



**Figure 5. Fourier transform of the spin correlations** in a high-symmetry plane of the frustrated pyrochlore magnet. Red regions denote strong correlations; black regions, weak ones. The local constraint on the sum over spins in a tetrahedron leads to the appearance of bow-tie motifs. These each have a pinch point at their center, which is a location of discontinuity but not divergence; the value of the spin correlations in the vicinity of those pinch points depends on the direction, but not on the distance, that one moves away from them. Back in real space, the ground-state constraint on the spins leads to algebraic correlations of the dipolar type,  $(3\cos^2\theta - 1)/r^3$ . (Courtesy of Sergei Isakov.)

essentially states that the residual entropy should vanish. In real, non-ideal systems, inevitable compound-dependent perturbations to the Hamiltonian lift the degeneracy unless the system freezes and falls out of equilibrium at low temperature anyway, a situation that appears to occur in spin ice.

One example of such a perturbation occurs in the sort of quantum dynamics that lifts the classical degeneracy in favor of the vacuum of artificial electrodynamics. Other examples include anisotropies, longer-range interactions, disorder, and spin–lattice coupling.

Such perturbations come with their own energy scale,  $v$ . Crucially, they cannot be treated perturbatively even if  $v/J \ll 1$ , because all the ground states have the same energy.  $J$  thus drops out as an energy scale. Frustrated magnetism is intrinsically nonperturbative.

Consequently, discovering the low-temperature state of the system can be quite difficult. Different perturbations will generally select different combinations of the unperturbed ground states as the temperature  $T$  drops below the energy scale of the perturbation. That is what makes the field of frustrated magnetism so rich from a materials science perspective. In the spin-liquid regime, though, where  $v \ll T < \theta_{\text{CW}}$ , many different frustrated magnetic compounds can look alike, each unstable toward its own low-temperature state.<sup>1,10</sup>

### Diagnostics

How can one tell if a material is geometrically frustrated? In real materials, geometrical frustration betrays its presence via the separation of energy scales,  $v \ll \theta_{\text{CW}}$ . As an example of a commonly used experimental diagnostic, we describe the susceptibility fingerprint of geometrical frustration.<sup>1</sup>

The magnetic susceptibility  $\chi$  measures the ratio of the magnetization to the strength of the magnetic field

applied to generate it. At high temperatures, the susceptibility follows the Curie–Weiss law—that is, its inverse is a straight line,  $\chi^{-1} \propto T - \theta_{\text{CW}}$ . For ferromagnets,  $\theta_{\text{CW}}$  is positive; for antiferromagnets, it is negative. In either case, mean-field theory predicts an ordering transition at temperature  $T_c \sim |\theta_{\text{CW}}|$ , and a corresponding anomaly in  $\chi$ , which is indeed observed for conventional magnets. The susceptibility curve in geometrically frustrated magnets, in contrast, remains smooth and stays close to the Curie–Weiss law, basically because the spins can continue to fluctuate almost as if they were free.

At a critical temperature  $T_c$  much lower than  $\theta_{\text{CW}}$ —that is,  $f \equiv \theta_{\text{CW}}/T_c \gg 1$ —frustrated systems typically are found to undergo a phase transition. The large value of  $f$  is therefore a simple consequence of the fact that the scale of  $T_c$  is set by  $v$ , whereas that of  $\theta_{\text{CW}}$  is set by  $J$ , so that  $f \sim O(J/v)$ .

The large size of  $f$  is not unique to geometrically frustrated systems. Low-dimensional systems also exhibit suppression of long-range order. But that effect need not be associated with a macroscopic residual entropy, which provides a simple diagnostic of the destruction of order due to frustration versus low dimensionality.

### A link to quantum Hall physics

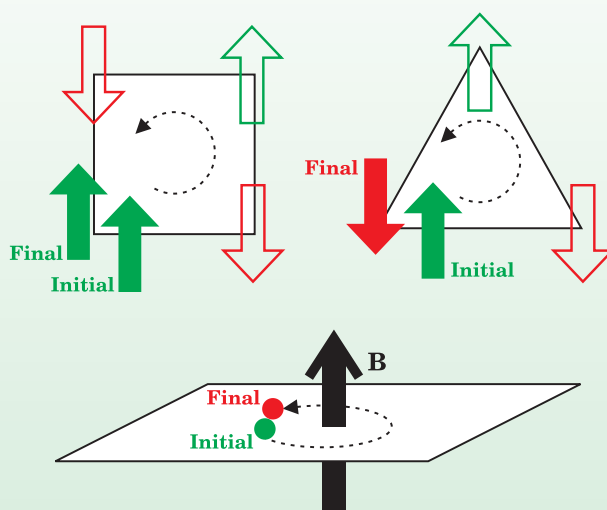
This article has explored the important role of degeneracies in magnetic systems. Another field in condensed matter physics in which they are prominent is the study of electrons in a 2D system immersed in a strong perpendicular magnetic field  $\mathbf{B}$ . In this quantum Hall regime, the energy levels of an ideal system form a discrete set of allowed values,  $\hbar v_c(n + 1/2)$ , where  $n \geq 0$  is an integer and  $\hbar v_c$  the cyclotron energy. To each  $n$  correspond many single-particle states grouped together in what's called the  $n$ th Landau level.

The connection between degeneracy and frustration relies on a notion of parallel transport. Imagine a spin that initially points up, say, being taken along an imaginary closed path around the lattice. The spin's orientation stays the same when its path crosses a ferromagnetic bond, and flips when it crosses an antiferromagnetic one. When the path closes, if the spin has encountered an odd number of antiferromagnetic bonds, the spin's final and initial states differ. That path is said to be frustrated (see figure 6).

Similarly, in quantum Hall physics, the wavefunction of an electron that crosses a closed loop of area  $A$  picks up a phase  $2\pi(AB/\varphi_0)$ , where  $\varphi_0$  is the flux quantum  $h/e$ . Unless the area  $A$  comprises an integer number of magnetic flux quanta, the final and initial states are again different. The difference is a manifestation of what can be termed a frustrated kinetic energy, which is ultimately the origin of the quantization into discrete Landau levels, each containing a macroscopic number of degenerate single-particle orbitals. (See the article by Joseph Avron, Daniel Osadchy, and Ruedi Seiler, *PHYSICS TODAY*, August 2003, page 38.)

The many ways of lifting the degeneracy of a Landau level give rise to the famously rich phase diagram of 2D electron systems, which exhibit zero-resistance states, fractionally charged quasiparticles, composite fermions, skyrmions, and charge-density waves. Similarly, the great richness of geometrically frustrated materials is related to the many instabilities of degenerate spin systems.

The search for other systems in which similar physics gives rise to unusual behavior is an exciting subject. One fascinating material, zirconium tungstate  $\text{ZrW}_2\text{O}_8$ , exhibits the peculiar structural property of having a lattice that shrinks when heated. Underconstraint in the material's lattice degrees of freedom, coupled with an unusual



**Figure 6. Frustration and quantum Hall physics.** Consider a spin, pictured as an arrow in the top panel, taken along some imaginary closed path in the lattice. It flips once for every antiferromagnetic bond encountered along the path. The bottom panel shows an analogous closed loop for an electron immersed in a magnetic field. In both the frustrated triangular lattice and the two-dimensional electron system, traversing the path leads to a final state that differs from the initial one: In the frustrated lattice the spin gets flipped, and in the 2D electron gas the phase of the electron wavefunction changes.

symmetry of the compound's vibrational modes, conspires to create this negative thermal expansion.<sup>11</sup> In many other materials, from metals to multiferroics, this unusual confluence of symmetry mismatch and underconstraint could play an important role in generating exotic properties. No doubt more will be found in the future.

We are grateful to Chanda Jog and Shivaji Sondhi for comments on the manuscript.

### References

1. A. P. Ramirez, *Annu. Rev. Mater. Sci.* **24**, 453 (1994).
2. L. C. Pauling, *The Nature of the Chemical Bond*, Cornell U. Press, Ithaca, NY (1945).
3. For a review of spin ice, see S. T. Bramwell, M. J. P. Gingras, *Science* **294**, 1495 (2001).
4. M. J. Harris et al., *Phys. Rev. Lett.* **79**, 2554 (1997).
5. A. P. Ramirez et al., *Nature* **399**, 333 (1999).
6. J. Villain, *Z. Phys. B* **33**, 31 (1979); I. Ritchey et al., *Phys. Rev. B* **47**, 15342 (1993).
7. O. Tchernyshyov et al., *Phys. Rev. Lett.* **88**, 067203 (2002); S.-H. Lee et al., *Nature* **418**, 856 (2002).
8. D. A. Huse et al., *Phys. Rev. Lett.* **91**, 167004 (2003); M. Hermele et al., *Phys. Rev. B* **69**, 064404 (2004); C. L. Henley, *Phys. Rev. B* **71**, 014424 (2005).
9. For a review of quantum frustration, see G. Misguich, C. Lhuillier, <http://arXiv.org/abs/cond-mat/0310405>; for a review of order in superconductors, see S. Sachdev, *Rev. Mod. Phys.* **75**, 913 (2003).
10. For an exemplary presentation, see H. Takagi, [http://online.kitp.ucsb.edu/online/exotic\\_c04/takagi/](http://online.kitp.ucsb.edu/online/exotic_c04/takagi/).
11. G. Ernst et al., *Nature* **396**, 147 (1998).