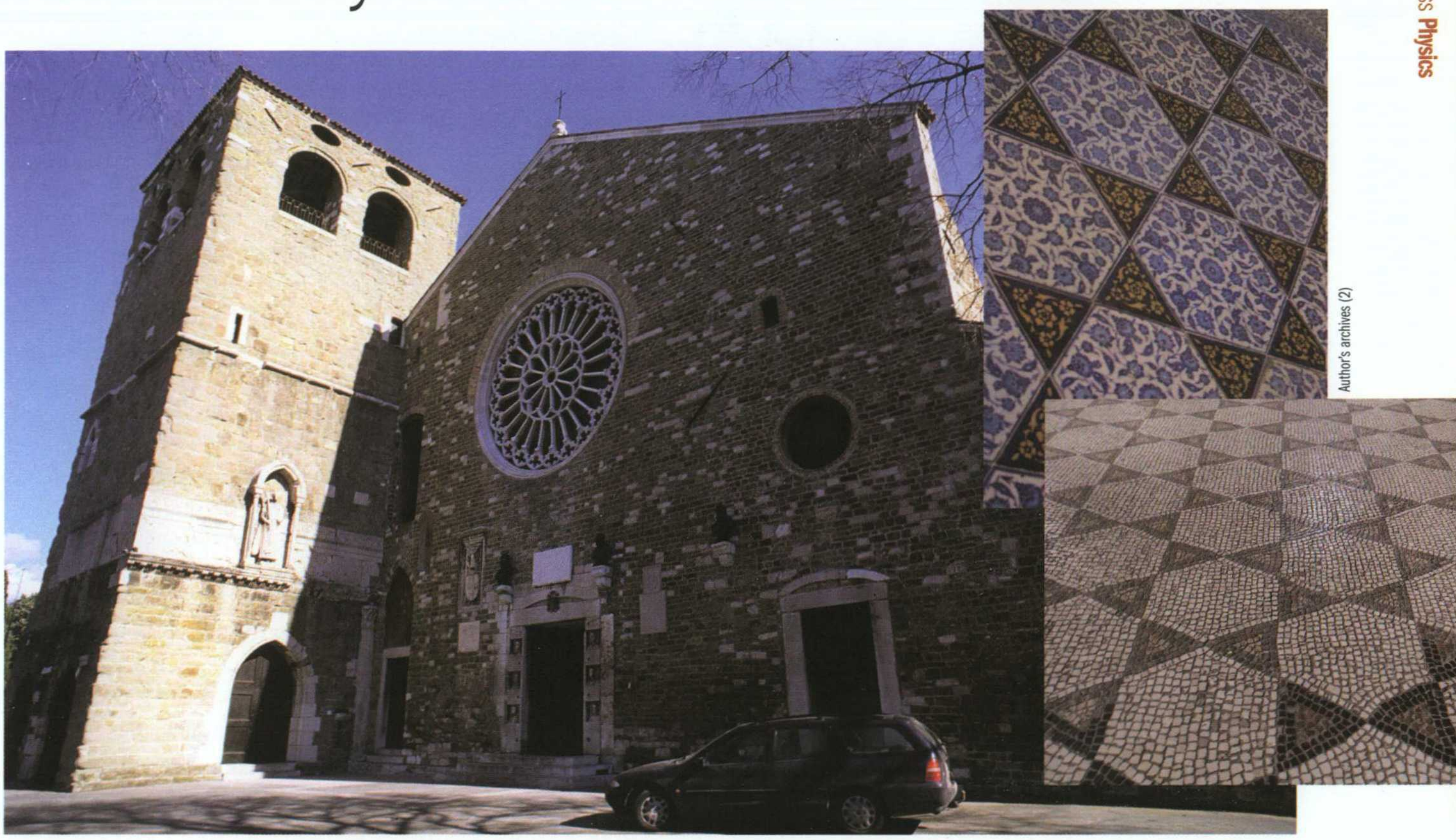
Can a Crystal Be Frustrated?



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One example of a two-dimensional frustrated lattice is the kagome (trihexagonal) lattice often used in medieval floor tile arrangements, such as at Trieste's Cathedral San Guisto

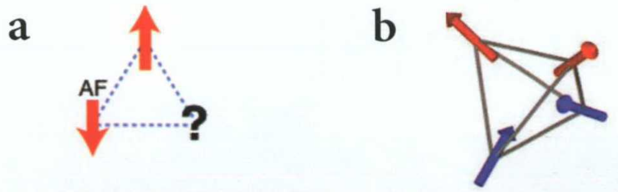
ANDRZEJ M. OLEŚ
Faculty of Physics, Astronomy and Applied Computer Science
Jagiellonian University, Kraków
a.m.oles@uj.edu.pl
Prof. Andrzej M. Oleś is the director of the Quantum Many-Body Theory Department.

Not being able to carry out our plans frequently leads to frustration. Can a similar phenomenon occur in physics? It turns out that it can

The notion is also applied to certain interacting magnetic moments. In certain situations, they cannot be arranged such that all pairs realize their favorable energy states. These situations are known as frustrated interactions, and the system is known as frustrated. Phenomena occurring in magnetic systems involving a conflict, or a frustration of interactions, are some of the most extensively studied and poorly understood problems of contemporary condensed matter physics. Rather than magnetic moments, physicists talk about spin, which acts similarly to a magnetic needle with one key difference: only two settings are possible (up or down). This is described in the Ising model, where the two spin states are denoted by an up or down arrow. A fundamental problem in frustrated magnetic crystals is the presence or absence of spin order.

Stressful geometry

The simplest frustrated spin system includes three spins interacting antiferromagnetically alongside the arms of a triangle in a way which favors opposite positioning for each neighboring pair. If the interaction between spins is antiferromagnetic, then in an ideal situation (in the absence of frustration) energy should be lower after each subsequent pair of opposite spins is taken into account. This is the case for four spins positioned at the vertices of a square and interacting along its sides, known as bonds. The situation is different for triangles: a state resulting in the minimum energy for each pair does not exist, and the energy for a system of three Ising spins is the same as the energy of a single

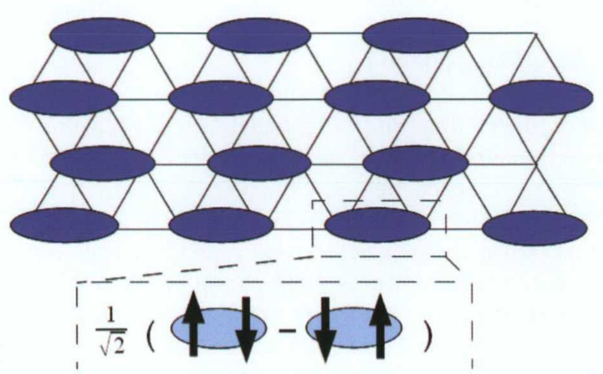


Frustrated spins with an antiferromagnetic interaction on a triangle (a). Positioning spins on a tetrahedron in spin ice – two-in-two-out state (b)

pair, because it is impossible to eliminate the defect of a pair of parallel spins. This type of frustration resulting from geometry is known as geometric frustration. An important property of frustrated systems is the high number of states with the lowest energy, or a high degeneracy of the ground state; for a single triangle, it has a value of six.

In systems described by quantum theory, discussing such states is insufficient, since spins are subject to substitution processes, and may fluctuate. The process leads to the lowering of energy, which is why the difference between the two configurations - the initial state and that resulting from switching spin orientation - is the ground state known as a singlet state of a pair of spins. The minus sign is significant, and it is the consequence of symmetry. In this instance, a system of three spins with antiferromagnetic coupling on a triangle is also frustrated.

Triangles placed next to one another and adjacent at the vertices form a triangular lattice. Another example of a two-dimensional frustrated lattice is the kagome or trihexagonal lattice commonly used to arrange mediaeval floor tiles, for example at the Trieste Cathedral. If quantum spins exhibit antiferromagnetic interactions, such systems are frustrated, similarly to three spins on a triangle. This raises the question of lowest energy states for spins exhibiting antiferromagnetic interactions in a triangular lattice. Unfortunately, for two-dimensional quantum spin systems it is impossible to give a precise answer to the question, because exact solutions are unknown. It is necessary to use approximate states, which may serve as a starting point in the search for a more realistic description taking into account quantum adjustments taking into account the nature of order or its absence for such systems of interacting spins.



Ordered state of quantum spin pairs (singlets) in a triangular lattice with antiferromagnetic interactions. The singlet (valence bond) is shown below. The energy of the system is the sum of the energy of all pairs

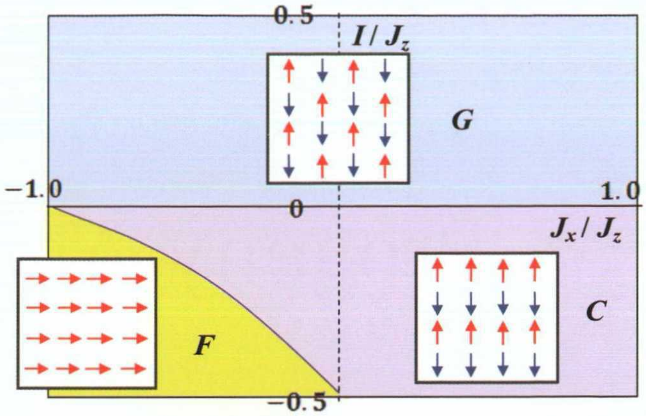
Ordered pairs

One possible low energy state is a state of ordered pairs of quantum spins (dimers), known as a valence bond state. The energy for each pair forming a singlet state is equal to the lowest possible quantum energy for a spin pair. A set of equivalent energy states with the shown system of singlets ordered in a single direction is very large, since the state of two neighboring and parallel singlets alongside two sides of a rhombus in a triangular lattice is equivalent to the singlets alongside the other two sides. This is why the degeneracy of the ground state is so significant. It also means that order is absent in the system, because all possible states must be considered at the same time.

When fluctuations between states with a different order of dimers within the lattice lead to the lowering of energy, we talk about the resonance of such states - a state without any order of spins or their pairs. A state in which quantum spins fluctuate and each possible spin state participates in such fluctuations is known as a quantum spin liquid. Fluctuations stabilizing such states also lead to reduced degeneracy, and it is frequently the case that the spin liquid state is nondegenerate, similarly to a quantum state of a spin pair (singlet).

Spin ice

Since a spin liquid state is possible for frustrated spins, it's worth asking whether a crystalline state or spin ice is also possible. Spin ice does indeed occur in three dimensions, in a lattice comprising tetrahedrons adjacent at the vertices known as a pyrochlore lattice in titanium oxides such as $Dy_2Ti_2O_7$. Magnetic ions of dysprosium (Dy) are found at the vertices of each tetrahedron. Due to the conflict of interactions in such a lattice, each tetrahedron contains two spins pointing inwards and two pointing outwards, giving the tetrahedron its total spin. Such spin states do not freeze at low temperatures and entropy remains finite, resembling ice crystals formed of water (H_2O). Linus Pauling noted that internal degrees of freedom exist in ice crystals, since two hydrogen atoms neighboring each oxygen atom are close to a single oxygen, forming the H_2O molecule, and the two remaining ones are further away. The number of such non-equivalent configurations increases rapidly with the increasing size of ice crystals; entropy remains finite for ice in the limit of zero temperature.

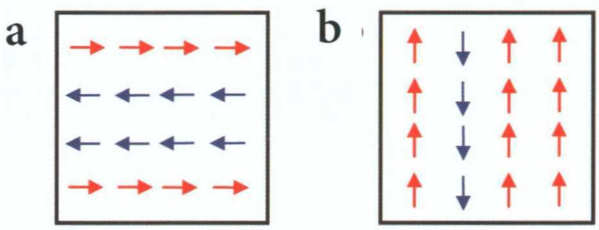


Phase diagram of the compass-Heisenberg model with Ising interactions Jx and Jz>0 along rows and columns of a square lattice. Ferromagnetic (F) and antiferromagnetic (G and C) states shown for a 4x4 cluster are formed as a result of quantum Heisenberg interactions, which eliminate frustration and destroy one-dimensional ordered states obtained in the compass model

Using spins interacting antiferromagnetically on a triangular lattice as an example, we note that frustration hinders the formation of ordered magnetic systems. In lattices without frustration, in which closed loops have an even number of bonds - such as in a two-dimensional square lattice - ordered states usually arise, either ferromagnetic or antiferromagnetic. This phenomenon is known as spontaneous symmetry breaking.

Frustrated spins

Frustration in a magnetic system may occur due to geometry, as encountered in the triangularlattice and pyrochlore examples; it may also result from the nature of interactions. Conflicts of interactions in square lattices also lead to fascinating states realized in condensed matter and in cold atom systems. Frustration on a square lattice is for instance realized by a compass model in which interactions are the same as in the Ising model, although they concern other spin components depending on the direction of the bond: x components along horizontal rows and z components along vertical columns in a square lattice.



One-dimensional spin configuration (arrows) in a ferromagnetic compass modal, with spins arranged: (a) along rows running left-right, or (b) along columns running up-down. changing the direction of all the spins along any given (a) row or (b) column leads to equivalent states with the same energy

This relationship of interaction with bond direction in a square lattice is the source of frustration occurring both for antiferromagnetic interactions and ferromagnetic interactions which prefer the same position of neighboring spins. To simplify somewhat, in such a system spins can be ordered only along rows or columns; as such, a one-dimensional (nematic) ordered system is realized, in which all spins are arranged either left or right alongside horizontal rows, or up or down along vertical columns. Errors in such ordered systems can be eliminated easily by orienting neighboring spins correctly, thus preserving information about the order. This is why such states may find application in quantum information transfer. Specific proposals exist of devices with protected qubits using a Josephson's vortex lattice, polar molecules or ion traps in optical systems.

A characteristic feature of frustrated systems is the ease with which the order of spins can be altered by an external field or an additional interaction. An example is the compass model, in which degenerate states with a one-dimensional order along one direction in a square lattice are replaced by a two-dimensional order, in presence of additional Heisenberg quantum interactions (hence the name compass-Heisenberg). Thus, such quantum interactions remove degeneracy and lead to spontaneous symmetry breaking within the entire two-dimensional lattice. In this situation, ordered systems can vary greatly. However, the secret of such systems is that the one-dimensional order of spins preferred by frustrated interactions survives in excited states with the lowest energies in nanoscopic systems, and it may be still used for quantum information transfer.

Another example of a frustrated spin system in a lattice with an even number of bonds for each closed loop is a hexagonal (honeycomb) lattice. In this instance, fascinating properties are exhibited by a generalized compass model (known as the Kitaev model), in which bonds in three different directions correspond to three quantum spin components. The model can be solved exactly, and its ground state is also a spin liquid state.

To summarize, conflicts of interactions in spin systems lead to disorder and large degeneracy of spin states. Such states arise when conflicting interactions balance one another and cannot induce any order. When the conflict disappears, other interactions - even weak ones - become significant and generate ordered states. This is how frustration in spin systems may lead to qualitatively new solutions. To return to our initial example, this resembles someone who has experienced severe stress and the resulting frustration; this likely gives a new perspective and experience which frequently provides a fresh look and leads to extremely valuable creative ideas. ■

Further reading:

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