The Undiscovered Potential of Magnetic Materials

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Thousands of years ago, magnetic lodestones were observed to attract certain metals such as iron at a distance. This mysterious phenomenon interested many people. While a scientific explanation of magnetism is now partly established, the potential of magnetic materials remains incompletely investigated. For example, “What is the strongest magnet?” sounds like a childish question, but we do not have an answer. A complete understanding of magnetism would allow scientists to predict the microscopic alignment of magnetic moments when only the atomic structure is given, but this is far from realization, and magnetism remains a major unsolved problem in condensed matter physics.

In the old days, ancient people described magnetism as a soul in the magnet or some invisible matter flowing between the magnet and the metal. As science developed, magnets could be described as a gathering of magnetic moments of electrons. Each electron has a magnetic moment, which behaves like a small magnet, and a state of magnetic moments aligned in the same direction is called a magnet, or, physically, a ferromagnet. Subsequently, scientists discovered magnetic states other than ferromagnetism [Figure (a)], such as antiferromagnetism (two adjacent magnetic moments that point in opposite directions) [Figure (b)], and ferrimagnetism (two adjacent magnetic moments that have different lengths and point in opposite directions) [Figure (c)].

For magnetic states to appear, interactions between electrons play a large role, and understanding them

are the largest barrier to an ultimate understanding of magnetism. If there were no interactions, magnetic moments would point in random directions and no magnetism would occur. Coulomb interactions and the Pauli exclusion principle, which prohibits two electrons from occupying the same state, have a tendency to align magnetic moments in parallel (same direction) or antiparallel (opposite directions) configurations. However, since a magnetic material of visible size has many electrons, on the order of the Avogadro constant ($\sim 6.0 \times 10^{23}$), it is almost impossible to solve the kinetic equation of these electrons including electron-electron interactions.

While a complete understanding is not yet achieved, physicists have managed to describe various magnetic phenomena theoretically and experimentally. Historically, the physics of magnetism developed by achieving theoretical explanations of experimentally observed magnetism. One major goal for theoretical physicists is to explain the sign (positive or negative) of magnetic interaction energy between magnetic moments, by which parallel or antiparallel alignments can be derived.

Magnetic interactions can be separated into several contributions: exchange interactions, superexchange interactions, and Dzyaloshinskii-Moriya interactions. Exchange interactions arise due to the antisymmetric properties of wave functions, which are a characteristic consequence of many-body quantum mechanics. Superexchange interactions were discovered to explain antiferromagnetism of MnO [1]. In MnO crystals, oxygen atoms are put between manganese atoms, and superexchange interactions occur indirectly via the non-magnetic atom (O) between two magnetic atoms (Mn). Dzyaloshinskii-Moriya interactions were derived by considering spin-orbit coupling in the discussion

of superexchange interactions and are responsible for a canted antiparallel order in α-Fe_2O_3 [2, 3].

Recently, numerical calculations by (super)computers have been another powerful tool to investigate magnetic materials. First-principle calculations such as density functional theory, which can perform calculations directly without any model for electronic states or wavefunctions, have predicted the properties of magnetic materials reasonably well. However, the calculation remains imperfect, since the interaction energy between electrons can be calculated only approximately.

Furthermore, the calculation power of computers is insufficient. If we assume the periodicity of the magnetic state to be the same as that of the crystallographic unit cell, the number of electrons considered decreases so much that we can easily calculate the magnetic property using first-principle calculations. The number of electrons in a unit cell is about 100, much smaller than that in actual materials (~10^{23}). However, the assumption of periodicity frequently fails, e.g. $CrNb_3S_6$ with chiral helimagnetic state, which has about a 40 times longer periodicity along the *c* axis than the height of the unit cell [Figure (d)] [4]. Moreover, some magnetic materials with characteristic properties are alloys or amorphous, which must have a longer periodicity even if we approximate the atomic structure. In both cases, first-principle calculations of magnetic materials have to be performed in a much larger temporary unit cell than the crystallographic one, and therefore require prohibitive calculation power.

As scientists have revealed the mystery of magnetic materials, little by little, through a collaboration of experiment and theory, established knowledge about magnetism has been applied to various kinds

of devices. This research field of applied physics is called “spintronics.” One famous application is the hard disk drive (HDD), which is a non-volatile data storage device installed in many computers. In the HDD, up-spin or down-spin states of one small magnetic domain represent 2-bit data (0 or 1), and these states are read or flipped using interactions with the magnetic head. Recent progress in spintronics has contributed to a higher recording density and larger capacity of the HDD. In this way, the accumulating knowledge about magnetic materials and magnetic physics will continue to develop, and will contribute to our lives and to society in the form of more powerful and convenient devices.

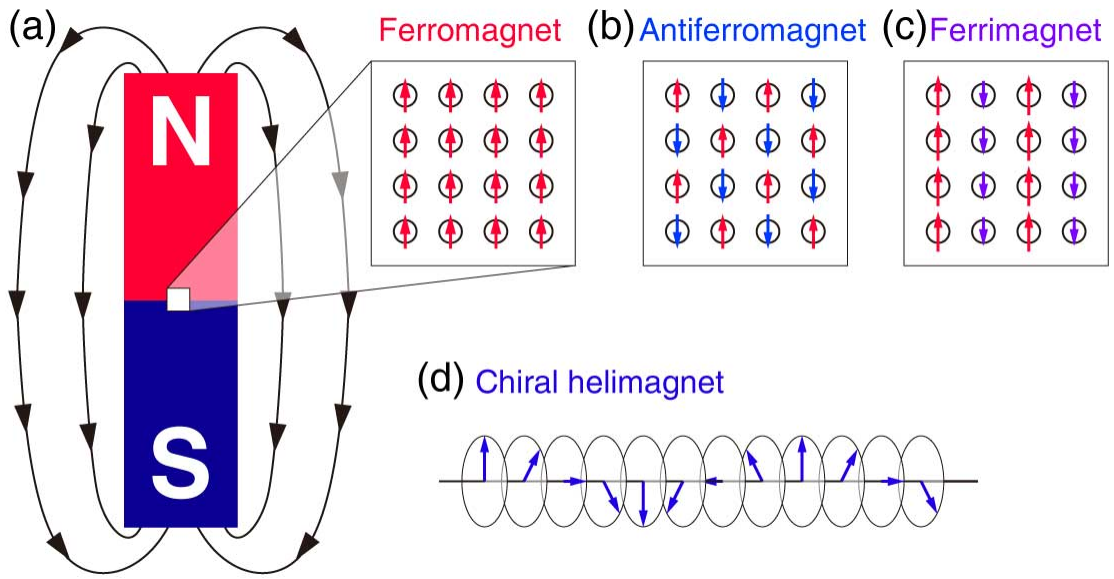

Figure: Schematics of a magnet and various magnetic states. In Figure (a), a schematic of a magnet and magnetic field lines are drawn. In the microscopic view, a magnet is composed of small magnetic moments of electrons pointing in the same direction. Two other magnetic states, antiferromagnetism and ferrimagnetism, are represented in Figures (b) and (c). Figure (d) represents the chiral helimagnetic state for $CrNb_3S_6$, in which magnetic moments form a helical structure along a horizontal axis.

References:

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