Modeling Tools for Magnetism, Magnetic Materials, and Spintronics: Overview

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Abstract

Spanning over a wide range of length and time scales, magnetism is one of the most fascinating states of matter and one that poses many challenges to theory. Here we briefly review how different state-of-the-art approaches to the modeling of the magnetic order interface with each other and provide a complete toolset to explore this fascinating area of condensed matter theory. Methods include accurate quantum-mechanical approaches, such as density functional theory both in its static and dynamical version, atomistic spin dynamics tools, and continuum models to be solved in a finite difference framework.

1 Modeling Magnetism

Magnetism is one of the most fascinating macroscopic orders of matter. It is deeply rooted in quantum mechanics and spans over many different scales in time, space, and energy (see Fig. 1). At its core magnetism is based on the m-J-κ paradigm. The Hund's coupling is responsible for the formation of the magnetic moment, m, often localized close to the atomic nuclei. This is active in open shell ions; hence

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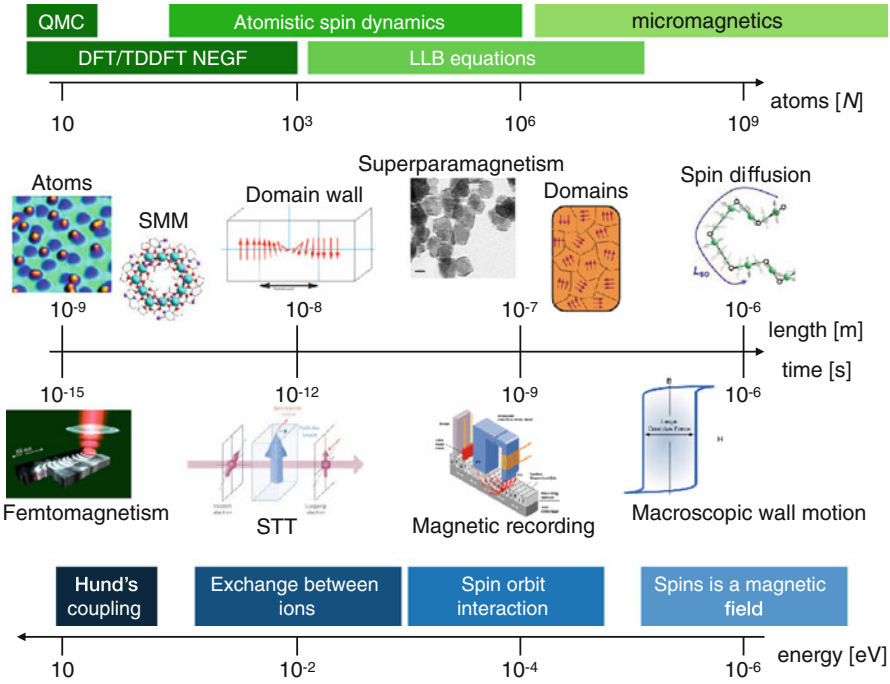

Fig. 1 Length, time and energy scales of magnetism. At the atomic level, the high-energy Hund's coupling is responsible for the formation of the local moments, which are then coupled to each other through exchange interaction. Finally, magnetic anisotropy aligns the moment along particular directions in space. The computational tools needed to explore and explain magnetism range from quantum mechanics-rooted methods, such as density functional theory (DFT) and Quantum Monte Carlo (QMC), to atomistic spin dynamics, and to effective theories allowing large-scale coarse graining, such as the Landau-Lifshitz-Bloch (LLB) and the micromagnetic approach

m forms in $2p$ radicals, among the elements in the $3d$ period, in rare earths and some $4d$ ions. Then the exchange interaction, J, makes the moments interacting with each other. At the microscopic level, a large variety of mechanisms is active in generating J at both sides of the metal/insulator boundary. These range from direct exchange to ion-mediated mechanisms and to those where the magnetic interaction is mediated by free electrons. Finally, the magnetic anisotropy, κ, is responsible for the interplay between spatial and spin degrees of freedom and ties the local moment to specific directions in space. The anisotropy, at the atomic level, is determined by the spin-orbit coupling.

The interplay and competition among the different interactions participating to the m-J-κ paradigm guide the formation of a multitude of magnetic orders. Locally exchange and anisotropy contribute to establish an alignment among the local moments, thus that often a microscopic order emerges. In simple cases, this can have the same periodicity of the crystal unit cell, but most frequently the crystal and magnetic cells are different. Then, classical magnetostatics imposes the formation

of macroscopically ordered regions (domains), separated by others where the order changes (domain walls). Symmetry breaking, for example through the presence of a surface, introduces additional complexity. In general the exchange and anisotropy get altered and, as a result, so does the macroscopic order.

Excitations of different energy can tip the various interactions and probe magnetism over many time scales. Intense, femtosecond-long, laser pulses interact directly with the electronic degrees of freedom (femtomagnetism). At this energy and time scale, the Hund's coupling, the exchange interaction, and the magneto-crystalline anisotropy are all functions of time, and the short-time dynamics is determined by their evolution. As time passes, the most energetic of the interactions, the Hund's coupling, returns m to its ground state value, meaning that the local moment recovers first. The dynamics is then determined by electronic currents interacting with local spins via exchange interaction. The same dynamics can also be engineered by passing spin-polarized electrical currents through magnets of various order. This is the realm of spin-transfer-torque devices. Now the exchange and the anisotropy are perturbed, and the magnetic order can be manipulated, both locally and globally. The energy scale of this phenomena is lower than that needed to alter the local moment, and the typical times vary between picoseconds and nanoseconds. In the slower limit of this range operates magnetic data storage technologies. Finally, when the dynamics is governed by macroscopic domain walls motion, magnetism slows down further, the exchange interaction becomes constant, and the time scale may approach the macroscopic range.

It is then clear that magnetism is both an atomic and a macroscopic phenomenon, and as such, it necessitates computational tools spanning a broad range of time and length scales. This chapter wishes to provide a map of the theoretical methodologies used to date to describe and understand the magnetic interaction.

At the atomic level, density functional theory (DFT) is usually the theory of choice, since it can describe all the interactions on the same footing and does not require any parameters from experiments. DFT for magnetism will be reviewed in ▸ Chap. 42, "Density Functional Theory for Magnetism and Magnetic Anisotropy" by Bihlmayer, while Friedrich, Müller, and Bluegel in ▸ Chap. 43, "Spin Excitations in Solid from Many-Body Perturbation Theory" will present how it can be applied to the description of magnetic excitations. Beyond-DFT methods usually require computational resources significantly larger than DFT itself. However, in some cases, they provide a more accurate description of both the moment formation and the exchange. Recent progress in Monte Carlo technique for d and f ions will be reviewed by Wagner in ▸ Chap. 46, "Quantum Monte Carlo for Electronic Systems Containing d and f Electrons". Finally, the DFT description of magnetism can be extended to time-dependent phenomena, as discussed by Elliott and co-workers in ▸ Chap. 40, "Time-Dependent Density Functional Theory for Spin Dynamics", and to open systems in the presence of a steady-state current, as described by Rungger and collaborators in ▸ Chap. 44, "Non-equilibrium Green's Function Methods for Spin Transport and Dynamics".

The next level of description is obtained by neglecting an explicit description of the electronic degrees of freedom. Namely, one can represent a magnet by

using local spins of constant magnitude associated to each atom. This provides an atomistic view of spin phenomena, at a course-graining scale analogous to that used in classical molecular dynamics for the ionic motion. These methods, reviewed by Ma and Dudarev in ▸ Chap. 47, "Atomistic Spin-Lattice Dynamics", can describe magnetic phase transitions for systems including up to several millions atoms and require parameters extracted either from experiments or from DFT calculations. Intriguingly, the interplay between the spin and the vibrational degrees of freedom can be described on the same footing. One can then integrate the dynamics over larger regions of space and move to a continuous description. This is the domain of micromagnetic methods, which allow to reach time and length scales approaching the macroscopic limit. The foundation of micromagnetic theory and and its connection to spintronics are discussed by Abert in ▸ Chap. 45, "Spintronics in Micromagnetics". In its most conventional form, only the transverse component of the magnetization can vary, while its longitudinal part is constant. However, a formalism based on the Landau-Lifshitz-Bloch equations allows to go beyond this approximation. Such range of methods is presented by Chubykalo-Fesenko and Nieves in ▸ Chap. 41, "Landau-Lifshitz-Bloch Approach for Magnetization Dynamics Close to Phase Transition".

2 Conclusion

We have briefly reviewed the state of the art in the modeling of the magnetic order both in the static and time-dependent domains. This develops over a range of computational schemes capable of bridging many length and time scales. In particular we have discussed the approximations that allow one to connect the various levels of theory, where a progressively smaller number of degrees of freedom are treated explicitly. Such a body of work gives us a complete toolset to tackle this fascinating area of materials science.

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References

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