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WHY WE LIKE MAGNETISM - WHY WE NEED MODELS - QUALITATIVE DESCRIPTION OF MODELS AND TYPES OF MAGNETISM

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Anyone who undertakes the organization of an advanced school (often called a summer school, irrespective of the season) must be very strongly motivated, or else totally inexperienced. We are fortunate to attend a school set up by experienced organizers, who knew very well the nature and amount of work involved and yet undertook the task. Good memories of schools attended as beginning researchers must be the most common motivation to do so, combined with the awareness of the need to bring a particular subject close to the new generation. The latter is the root of the first question I have been asked to answer.

Why Magnetism?

Magnetism is a very wide subject, expanding over physics, chemistry and materials science, and intruding into the life sciences. In the past decades it has undergone rapid developments, in particular in three areas with actual or potential applications:

- Permanent magnets (electro motors),
- Thin films (data storage, writing and reading),
- Nano particles (ferrofluids, medical applications).

There is still intensive research and development work in progress on these subjects. Most of this work entails the application of phenomenological, often classical description of specific processes and constructions. On the other hand challenging problems, both conceptual and theoretical, remain open. In fact, these are in the focus of the program of ESM2009. This statement seems to contradict the title of the school, “Models in Magnetism”. Hence the second question I am supposed to answer.

Why Models?

Magnetism is an immensely complex subject. Sometimes I think I should have run away when I heard the absurdity that you cannot cut off the North Pole of a magnet, you will walk away with a North and a South poles in your pocket anyway. This was at high school, later, having handled some classical models (Langevin); we have also learned that there is no magnetism in classical physics. It is not for nothing that Niels Bohr has attacked this problem, the result being the Bohr – van Leeuwen theorem that says that a system of charged particles obeying classical mechanics has zero magnetic susceptibility. For some reason, in most textbooks this is stated in connection with diamagnetism, but there is no such limitation on the theorem's validity. Surely, without the quantisation of angular momentum, a charged particle has no stable orbit around a point charge of opposite sign.

The Bohr atom, with its classical electrons obeying angular-momentum quantization, allows for atomic magnetic moments. Quantum mechanics also allows the determination of the current density generated by electrons in various orbits, using Schrödinger's equation. But we again bump in a limitation, when we try to convert this into a spatial distribution of the magetisation within the atom, which is supposed to be given by the differential equation $\nabla \times \mathbf{M} = \mathbf{j}$. Where we have learned that $\nabla \times \mathbf{A} = \mathbf{B}$ does not determine the vector potential, because of the gauge freedom, the same limitation is seldom pointed out about the analogous relation between **M** and **j**. Inside an atom, only the magnetisation due to the electron spin can be calculated, it is proportional to the spin density. But then, we are stuck with the problem of a point-like particle spinning and we have to go further, to the Dirac equation to accept that the electron has to have a spin. All this is supposed to illustrate the complexity of magnetism. We *accept* the outcome of relativistic quantum mechanics, which is different to *understanding* with an "Aha!" experience and a feeling of "I see". We do not see an atom, not even a magnetic nanoparticle, not even with a microscope.

The vector model

This is where the models come in. Already in atomic physics, the consequences of the spin-orbit coupling, which is a relativistic effect, are described in terms of the vector model. This model is helpful in the description of Hund's rules, a cornerstone in localized-moment magnetism. It is also implicitly used in crystal field theory, which provides a framework for a discussion of the coupling of the magnetisation to the crystal lattice.

Spin Hamiltonians

Localized moments serve as the basis for a large number of models of the cooperative effects, i.e. magnetic ordering and spin waves. Such models are defined by spin Hamiltonians, in which the interaction of localized moments is represented by products of angular-momentum operators. It is remarkable, how successful these models have been throughout half a century while heated discussions were going on about the existence of localized moments. Likewise, the itinerant-electron model was developed to a high degree of sophistication in the same period. Numerical work, band-structure calculations, entered magnetism in this connection. This has limited the possibilities to explain particular experimental results. To fit such results, it is often possible to find a density of states function that will do the job. Reliable independent density of states curves can make this impossible, enabling at the same time the identification of the breakdown of simple itinerant-electron behaviour.

Modelling the exchange coupling between localized moments

In the models mentioned above, the interaction between magnetic moments is parameterized in the simplest possible way. About the physics behind the interaction it is clear that magneto static interactions are unimportant. Heisenberg showed that the exchange interaction can explain ferromagnetic ordering, but the discovery of antiferromagnetic ordering called for more sophisticated calculations. Various mechanisms have been identified to explain antiferromagnetic exchange and even anisotropic exchange, which involves, apart from the angle between the two interacting spins, also the spin orientations with respect to the vector connecting the two localized moments. The models used in the calculation and verbal description of the exchange interaction are formulated in terms of a limited number of localized states on each atom or ion and again a limited number of matrix elements between such states. These are of two kinds, matrix elements of single-particle and two-particle operators. Of the former, most important is the "hopping term" t, which describes what it says: the transition of an electron to a neighbouring localized state. Of the latter, the "Hubbard U" is the most important, which stands for the Coulomb repulsion between two electrons occupying the same orbital state, with opposite spins. As can be expected in second-order perturbation theory, this so-called super-exchange coupling is of the form $|t|^2/U$. Such a two-parameter theory is of course too sketchy. Localized magnetic moments involve d or f states, for which there are five and seven wave functions, respectively. To explain the observed

variation of the exchange coupling in different geometries, the models have to be enriched with more localized states and new parameters. Here too, the emergence of numerical work has limited the possible combinations of parameter values, eliminating "wishful thinking" in the efforts to account for all observations.

The hopping term t is of course the same matrix element that we know from the tight-binding approximation of Bloch wave functions. Naturally, if hopping is possible from an atom to its first neighbour, it will be also possible from the first to the second neighbour and so on. This identification leads us to the limit of the validity of the model underlying super-exchange. The formula found in second order in the hopping term suggests that to get a strong exchange coupling, we should look for materials with large values of t. But surely, that will give a mobility to the electrons that disqualifies the localized-electron model and leads us back into the world where the itinerant-electron model is appropriate. This is not a sharp distinction. Between the two models is the most challenging area of magnetism.

Deceptively simple-looking models

The term "strongly correlated electron systems", which describes this area can be taken for a warning: forget about mean-field theories. The models used to describe these systems *look* simple, but hide a gold mine of possible phenomena. How well the gold is hidden can be illustrated with the Kondo Hamiltonian. It is the simplest Hamiltonian one can think of for the description of a localized electron in the sea of free, non-interacting electrons. Yet it took sixteen years to solve the Kondo problem. Likewise, the Hubbard model, which was designed to elucidate the itinerant vs. localized duality in 3d transition metals, but actually is more relevant to oxides, where there is no conduction band in the energy range of interest, is stripped from all parameters except t and U and the particle density, nevertheless exact results are only available for specific values of the parameters. Yet, there is progress in the understanding of strongly correlated electron systems and of the phenomena observed in these systems, such as non Fermi liquid behaviour, quantum criticality and coexistence of ferromagnetism and superconductivity.

Phenomenological models

Processes involving domains and domain walls are commonly described in phenomenological models. Unlike the models dealing with exchange interactions, in which the state of the electrons are treated quantum mechanically and spin Hamiltonians, where

atomic moments are treated classically or quantum mechanically, the models used to study magnetisation processes, hysteresis loops and switching ignore the atomic structure and treats magnetisation as a continuum. Only the symmetry properties of the crystal lattice are used to determine the nonvanishing terms in the anistropy energy. Although reliable ab initio calculations of the anisotropy constants are beginning to appear, it is more common to determine these parameters experimentally. The thickness of multilayers is diminishing every year, but continuum models are still popular, where for the propeties of layers (magnetisation, anisotropy, electrical conductivity) the bulk values are used.