Theory of d-zero and low-dimensional magnetism

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1. Background and purpose of proposed research period

My research activity has been in the field of theoretical condensed matter physics, particularly in low-dimensional quantum magnetism. In my earlier work this involved the developments of numerical renormalization group methods based on exact diagonalization. I have had a continued interest in the static and dynamic correlation functions of magnetic materials that can be studied by neutron scattering, and have collaborated with experimentalists in this field. More generally I have been involved in the interpretation of experiments in high magnetic fields, both static and, most recently, dynamically generated, one of the specialities of the IMR. Frustrated magnetic systems in one and two dimensions have been particularly interesting as the frustration may lead to exotic ground states such as spin liquids. Spin-orbit interactions and resulting Dzyaloshinsky-Moriya couplings can play an important role in the dynamics of frustrated systems, for example in allowing transitions otherwise forbidden by symmetry and in producing multi-functional materials.

In recent years I have developed an interest in diluted magnetic semi-conductors and so called “d-zero” magnetism. Here the samples are normally films and the experimental situation is much less established than in bulk magnetic system. It is therefore a particular challenge to understand the physics, but there is the motivation of the possible applications in spintronics. An exciting area is that of “nano-magnetism”, i.e. of the properties of nano-scaled molecules in isolation or weakly coupled in molecular solids. This is both for potential application and conceptually important, in that the properties of dissipation coming from in coupling to the environment become central to their properties.

2. Proposed plan

In the search for novel materials, with combinations of magnetic and semiconducting properties potentially useful for spintronics applications, a new approach is to look at systems where there may be magnetic moments induced by impurities or defects, but with no d- or f-shell electrons. This is known as d0 magnetism to indicate that the magnetic moments reside in p-orbitals, of oxygen (or of carbon or nitrogen...) Last year, I had collaborated with Prof. Maekawa's group to understand possible observation of ferromagnetism in films of magnesium oxide doped with nitrogen[1]. Another new system is that of NV centers in diamond. A single center, a nitrogen impurity bound to a carbon vacancy, has a magnetic moment shown to have long quantum-mechanical coherence times even at room temperature. There is interest in exploiting this for making interacting qubits. It is important to understand interactions between different impurities. The plan for the visit as guest professor at the ICC-IMR in the group of

Professor Maekawa was particularly to further the theme of d^0 magnetism by looking at other candidate materials and dopants and to calculate the interactions between impurity-induced moments using quantum Monte Carlo methods developed previously.

We also wished to adapt the previous calculational methods to predict interactions between different centers. This should enable predictions of magnetic properties of finite concentrations of centers. Measurements of coherence have given detailed information on the hyperfine couplings responsible for relaxation of isolated impurities. By adapting calculations made to interpret relaxation effects in triangles of spin ½ in molecular nanomagnets (in the group of Prof. Nojiri at IMR) to small clusters of NV centers, we should also be able to predict coherence properties of these clusters.

3. Results and discussions

In the proposed theme of d^0 magnetism, part of the effort was devoted to developing a microscopic model for predicting the interaction of negatively charged V-N centers in diamond. This formulation is at the basis of new calculations to be conducted with Prof. Maekawa’s group in the future. I also joined in a theoretical project that had been started previously in the group, following the discovery in the IMR of a giant spin Hall effect at room temperature in a device with injectors made of Iron Platinum alloys and a Gold cross bar[2]. One of the fundamental bottlenecks in developing spin electronics is to find mechanisms that allow electrical currents to convert efficiently to spin currents. Thus this discovery of giant spin Hall effect may be crucial to the development of spintronics and must be understood. A qualitative theory had been advanced by Guo et al [3] explaining this surprising result in terms of resonant skew scattering by individual Fe atoms in the Au host. The scattering by spin-orbit coupling is enhanced by Kondo-type many body interactions even at room temperatures, because the crystal field splitting leads to an orbital Kondo effect with a high temperature scale in addition to the standard Kondo temperature, below 1K, coming from the strongly coupled crystal field levels. The original predictions of Guo et al [3] relied on band structure calculations which must be supplemented by techniques that fully include many-body fluctuations of strongly correlated electrons. In recent numerical studies [4], Quantum Monte Carlo methods have been applied which supported this interpretation and gave quantitative predictions down to room temperature. Nevertheless important questions remain, particularly as concerns consistency with measurements of transport and orbital magnetism performed at low temperatures on systems close to the model proposed: *i.e.* dilute alloys of Fe in gold.

In parallel with this work, my visit to the IMR was instrumental in establishing a collaboration in the area of low-dimensional magnetism with ICC visiting Professor Seung-Hun Lee, of the group of Prof. K. Yamada, who was analysing neutron scattering data on a spatially anisotropic triangular antiferromagnet Ag_2MnO_2. Their results showed that the compound shows a freezing transition at low temperatures to an unusual phase of short-range collinear order but gapless fluctuation spectrum. My contribution was in theoretical interpretation of the results in terms of a spin liquid phase that have been postulated for an anisotropic triangular antiferromagnet[5].

4. Summary and perspectives:

As one of the goals is to suggest alternate materials to make devices with useful spin Hall effects, the calculations should be extended to consider other possible impurities, transition metals or rare earths as suggested by Guo et al, and other “hosts”, i.e. choices of metals for the Hall bar. There are also fundamental questions concerning the cross-over between very low temperature properties and the room temperature transport which should clarify the scaling properties of spin-orbit couplings, crystal field splitting and Hund's rule coupling in a temperature range between the low temperature Kondo temperature and the higher temperatures of the orbital Kondo effect. These can be studied by Quantum Monte Carlo techniques and compared to results from Numerical Renormalization Group at low temperatures. At the same time, there remain difficulties in reconciling this model and other experimental results on impurities, in particular measurements of orbital angular momenta by X-ray Magnetic Dichroism. In this work [4] a resolution was proposed, based on numerical results that indicated that as a function of magnetic field there could be a transition between a high orbital moment state with high skew scattering and a low moment state with weaker scattering. The separation between the two regimes depends on the exact hybridization and (exchange) field seen on the d-ion so that it could be strongly influenced by small changes in the environment. The results open up the perspective of making more systematic studies of orbital magnetism, in collaboration with experimental groups at the ESRF in Grenoble and Spring-8, Himeji, using X-ray MCD to look at effects of environment on the measured orbital moments: for example the proximity of other Au atoms or Pt atoms in the FePt alloy that composes the electrodes and the depth dependence of orbital magnetism close to interfaces of Au and FePt.

References:

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