Theoretical modelling of magnetic phase diagrams and interpretation of experimental data.

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In this project we will investigate how to model theoretically magnetic properties of materials. We will use the calculations that result from the theoretical work both to analyse experimental measurements and also to feedback the information from experiment to improve further the theoretical models.

Models of magnetic materials are usually expressed in terms of many interacting *spins* associated with atomic positions. Hamiltonians containing a number of terms. They interact with each via *exchange interactions*, are affected by *crystal fields* and *spin-orbit* coupling which depend on the geometry and nature of the atomic and electronic environment, and with applied magnetic fields via a *Zeeman* term [1,2].

We will use a simple model, with a mean field approximation for the statistical mechanics of the spins, to describe a magnetic phase diagram. The parameters for such models can be extracted from experiment and how the models can help interpret and analyse experimental data. To do this we will use the established *McPhase* computational package. [3,4]

The program package McPhase has been developed in order to calculate static and dynamic magnetic properties of rare earth compounds in particular. Crystal field and exchange parameters are required as an input for the calculations. A mean-field calculation is repeated with randomly chosen initial spin configurations in order to determine the most stable magnetic structure at a given temperature and magnetic field. By subsequent calculations at several temperatures and magnetic fields a magnetic phase diagram can be mapped. Using a special module of the program package the input parameters may be varied in order to find a model description, which corresponds to experimental data.

Geometrical frustration is a general concept employed to describe the properties of various systems in which the magnetic interactions are incompatible with the underlying lattice geometry. Often such systems are unable to form a unique ground state with a conventional long-range order and therefore display a particularly rich variety of unusual phenomena related to magnetic frustration at low temperature. The Superconductivity and Magnetism Group at Warwick [5] has a long history of studying such materials. This project will analyse the Group's experimental data on the compound $Co_3V_2O_8$ which is known to adopt a buckled version of the Kagome lattice, called the Kagome staircase. This compound possesses a very complex magnetic phase diagram where the sequence of the phase transitions is of particular interest. Intriguing magnetic excitations have been observed by our group using inelastic neutron scattering measurements [6]. In this project we will find a theoretical model to interpret these neutron scattering data and determine the nature of the magnetic interactions.

[1] *Introduction to Magnetism and Magnetic Materials*, D.C.Jiles , Chapman and Hall (1998).

[2] *Rare Earth Magnetism*, J. Jensen and A. R. Mackintosh, Clarendon Press Oxford (1991).

[3] McPhase Package: http://www.cpfs.mpg.de/~rotter/homepage_mcphase/McPhase_-_the_World_of_Rare_Earth_Magnetism.html

[4] M. Rotter, J. Mag. Magn. Mat., 272, E481-2, (2004).

[5] http://go.warwick.ac.uk/supermag

[6] N. R. Wilson *et al*., J. Magn. Magn. Mater. **310**, 1334 (2007); N. R. Wilson, PhD Thesis, Warwick 2007.