The Influence of Confinement on Phase Transitions (Part 1)

Report of Contributions

https://indico.fysik.su.se/e/1136

Contribution ID: **251** Type: **not specified**

Introduction and Setting the Stage

Monday, February 15, 2010 11:00 AM (1 hour)

Give a thorough description of the experimental results
concerning dimensionally confined magnetic systems.

Primary author: Prof. HJÖRVARSSON, Björgvin (Uppsala University)

Presenter: Prof. HJÖRVARSSON, Björgvin (Uppsala University)

Contribution ID: **252** Type: **not specified**

Confinement and Ordering

Tuesday, February 16, 2010 1:00 PM (1 hour)

Primary author: Prof. HOLDSWORTH, Peter (Ecole Normale Supérieure de Lyon)

Presenter: Prof. HOLDSWORTH, Peter (Ecole Normale Supérieure de Lyon)

Contribution ID: **253** Type: **not specified**

Phase Transitions and Critical Phenomena

Wednesday, February 17, 2010 2:00 PM (1 hour)

Primary author: Prof. BRAMWELL, Steve (University College London)

Presenter: Prof. BRAMWELL, Steve (University College London)

Contribution ID: **254** Type: **not specified**

Dipolar Systems

Thursday, February 18, 2010 2:00 PM (1 hour)

Due to the long range and angular dependence of the dipolar interaction sample shape plays a crucial role in determining the ordered state of magnetic materials where long-range interactions are important. This should also apply to magnetic mulitlayer systems and I propose studying the effects of the often neglected dipolar interaction in these novel materials.

Primary author: Prof. HENELIUS, Patrik (KTH Royal Institute of Technology)

Presenter: Prof. HENELIUS, Patrik (KTH Royal Institute of Technology)

Contribution ID: **255** Type: **not specified**

Critical Temperatures of Finite Samples at Finite Observation Times

Monday, February 15, 2010 2:00 PM (1 hour)

The correlation function is an essential ingredient of any theory of phase transitions, covering electronic systems, liquids or magnets, since it provides direct information on critical properties of a system. With the Ornstein-Zernike law its general analytical form is known for infinite systems at infinite observation times, above the critical temperature.

However, important experimental developments involve ever smaller length- and time-scales connected with size- and time-dependent phases like thermally assisted switching of magnetization. For such nano-sized systems, there is up to now no clear understanding of crossover phenomena like the crossover from a paramagnetic state at high temperatures via a superparamagnetic regime to ferro- or antiferromagnetic order at low T, and how they manifest themselves in the correlation function. This is related to the problem that a Curie (or Neel) temperature cannot be defined unambiguously. These problems hamper a reliable interpretation of experimental results.

In this talk I will present a particularly simple general expression for the correlation function, covering all sample sizes L, all observation times, and the entire temperature range from zero to infinity. Our numerical and analytical calculations demonstrate that the Curie temperature does not simply decrease with decreasing sample size but rather splits in finite samples for finite observation times. This new result obtained for open boundaries does not violate scaling invariance and recovers all known laws for periodic boundary conditions, infinite observation times and high temperatures as limiting cases. The proposed form for the correlation function allows for a novel and effective procedure to determine above mentioned splitting and critical temperatures which goes beyond the famous Binder cumulants method as it permits an accurate determination of the Curie temperature of infinite and finite objects, as well as the blocking temperature, from a single calculation of a finite object without tedious finite-size scaling.

Primary author: Dr VEDMEDENKO, Elena (University of Hamburg)

Presenter: Dr VEDMEDENKO, Elena (University of Hamburg)

Contribution ID: **256** Type: **not specified**

Structure modifications in ultra thin films of transition metal oxides

Wednesday, February 17, 2010 11:00 AM (1 hour)

The talk reviews recent studies on the geometric structure of oxide films in the ultra thin film limit and their implications on their magnetic (multiferroic) properties. In a first example the structural phase transition in pure and Cobalt-doped ZnO-film is discussed. Depending on film thickness a transition from the bulk Wurtzite (WZ)-type structure to the hexagonal-Boron-nitride (h-BN) phase is observed. Cobalt doping leads to a phase segregation in which WZ-type CoO-nanoclusters are coherently embedded into the h-BN host ZnO matrix. The structure model involving locally confined antiferromagnetic CoO-clusters supports recent experimental results on the magnetic properties of diluted magnetic semiconductors. The effect of confinement is also decisive for the multiferroic (ferromagnetic/ferroelectric) properties of the BaTiO3/Fe(001) interface, which is addressed in the second part of the talk. The structure analysis in combination with first principles calculations reveals the onset of an interface dipole at a critical film thickness of two unit cells of BaTiO3. Its influence on the magnetoelectric properties is discussed.

Primary author: Dr MEYERHEIM, Holger (Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany)

Presenter: Dr MEYERHEIM, Holger (Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany)

Contribution ID: **257** Type: **not specified**

Magnon Softening in a ferromagnetic monolayer

Tuesday, February 16, 2010 10:00 AM (1 hour)

We study the Fe/W(110) monolayer system through a combination of first principles calculations and atomistic spin dynamics simulations. We focus on the dispersion of the spin waves parallel to the [001] direction. Our results compare favorably with the experimental data of Prokop et al. [Phys. Rev. Lett. 102, 177206], and correctly capture a drastic softening of the magnon spectrum, with respect to bulk bcc Fe. The suggested shortcoming of the itinerant electron model, in particular that given by density functional theory, is refuted. We also demonstrate that finite temperature effects are significant, and that atomistic spin dynamics simulations represent a powerful tool with which to include these.

Primary author: Dr BERGMAN, Anders (Uppsala University)

Presenter: Dr BERGMAN, Anders (Uppsala University)

Contribution ID: **258** Type: **not specified**

Quantum critical points via gravity

Wednesday, February 17, 2010 3:00 PM (1 hour)

Primary author: THORLACIUS, LÃ¡rus (Nordita)

Presenter: THORLACIUS, LÃ¡rus (Nordita)

Contribution ID: **259** Type: **not specified**

The effect of geometric constraints on the spin glass transition in binary pyrochlores

Thursday, February 18, 2010 10:00 AM (1 hour)

Recent neutron scattering experiments [1] have sharpened the picture of an algebraic spin liquid phase in CsNiCrF6, originally proposed by Zinkin et al. [2]. Anderson famously predicted that systems such as this, with equal numbers of two magnetic species populating a pyrochlore lattice, should favour configurations with two of each type of ion present on every tetrahedron [3].

With this in mind, we have studied a simple model of a system comprised of equal numbers of two species of Heisenberg spins, A and B, distributed randomly across a pyrochlore lattice, but subject to the ice-rules like constraint that each tetrahedron has two A and two B type spins. We have characterized the ground state magnetic behaviour for all possible combinations of the three exchange interactions governing the system. This reveals a large region of exchange parameter space for which the system is in a spin liquid like state consisting of a soup of single species, non-interacting, antiferromagnetic loops. This configuration is robust even in the presence of four ferromagnetic bonds per tetrahedron. We demonstrate that the highly constrained form of quenched disorder imposed on the ion placement removes the possibility of a spin glass transition from this cooperative paramagnetic regime. We go on to discuss how the underlying structural configuration leads to algebraic magnetic correlations, manifested in the familiar bow-tie structure factor. This model is also susceptible to strong finite size influences. A system with finite size will be unable to develop the correct loop distribution to produce the bow-tie structure factor. We are currently investigating how such effects manifest themselves and the implications for more controllable arrays such as can be achieved with, for example, artificial spin ice.

[1] T. Fennel et al., unpublished.
[2] M. P. Zinkin et al., Phys. Rev. B 56, 11786 (1997)
[3] P. W. Anderson, Phys. Rev. 102, 1008 (1956)

Primary author: Dr BANKS, Simon (University College London)

Presenter: Dr BANKS, Simon (University College London)

Contribution ID: **260** Type: **not specified**

Phase transitions with disorder

Thursday, February 18, 2010 11:00 AM (1 hour)

Disordered systems often display new emergent phases and phase transition, for example, spin glasses and similar states in quantum fluids with disorder. Other examples where confinement effects play an important role are given by porous matter. Experiments on such systems often indicate strong finite size effects that need to be understood. We use an approach involving Monte Carlo simulation and scaling analysis to address these issues. I will describe some of our recent studies.

Primary author: Prof. WALLIN, Mats (Theoretical Physics KTH)

Presenter: Prof. WALLIN, Mats (Theoretical Physics KTH)

Contribution ID: **261** Type: **not specified**

Methods in simulations

Thursday, February 18, 2010 3:00 PM (2 hours)

Contribution ID: **262** Type: **not specified**

Magnetricity in Spin Ice

Friday, February 19, 2010 1:15 PM (1 hour)

Primary author: Prof. BRAMWELL, Steve (University College London)

Presenter: Prof. BRAMWELL, Steve (University College London)

Contribution ID: **263** Type: **not specified**

Hunting for monopoles in spin ice

Friday, February 19, 2010 10:15 AM (1 hour)

Primary author: Prof. HOLDSWORTH, Peter (Ecole Normale Supérieure de Lyon)

Presenter: Prof. HOLDSWORTH, Peter (Ecole Normale Supérieure de Lyon)

Contribution ID: **264** Type: **not specified**

Future Perspectives

Friday, February 19, 2010 3:00 PM (2 hours)

Contribution ID: **265** Type: **not specified**

A family of critical models in d-dimensions

Monday, February 22, 2010 1:15 PM (1 hour)

It is well known that the order parameter for the 2dXY model is zero in the thermodynamic limit, yet it remains measurable even for macroscopic systems. Thus our ability to observe the KT transition via changes in the magnetization is a result of the "confinement" of the system to finite size. We have been working on a family of related models in one and three-dimensions generalizable to d-dimensions) which exhibit behaviour closely analogous to the 2dXY model. We will consider the possibility that confinement in these models may lead to KT type, or possibly other novel, phase transitions.

Primary author: Dr BANKS, Simon (University College London)

Presenter: Dr BANKS, Simon (University College London)

Contribution ID: **266** Type: **not specified**

The p,q-binomial distribution applied to the finite-size Ising model

Monday, February 22, 2010 2:15 PM (1 hour)

Primary author: Dr LUNDOW, Per Håkan (KTH Royal Institute of Technology)

Presenter: Dr LUNDOW, Per Håkan (KTH Royal Institute of Technology)

Contribution ID: **267** Type: **not specified**

Simulation of long time scale evolution in solids

Tuesday, February 23, 2010 10:15 AM (1 hour)

Primary author: Prof. JONSSON, Hannes (University of Iceland)

Presenter: Prof. JONSSON, Hannes (University of Iceland)

Contribution ID: **268** Type: **not specified**

Magnetic X-ray scattering (part I)

Tuesday, February 23, 2010 1:15 PM (1 hour)

Primary author: Dr HASE, Tom (University of Warwick)

Presenter: Dr HASE, Tom (University of Warwick)

Contribution ID: **269** Type: **not specified**

Phase Transitions and Dimensionality

Wednesday, February 24, 2010 10:15 AM (2 hours)

Primary author: Prof. STINCHCOMBE, Robin (University of Oxford)

Presenter: Prof. STINCHCOMBE, Robin (University of Oxford)

Contribution ID: **270** Type: **not specified**

First principles theory of magnetism and magnetisation dynamics

Wednesday, February 24, 2010 1:15 PM (1 hour)

In the talk I will review some recent results on first principles theory of magnetism and magnetic materials. In particular, results of giant magnetic anisotropies will be described, and I will put some emphasis on technological aspects of this property. I will also describe recent developments in theory of spin-dynamics and how this reproduces observations on thin-film magnetism, diluted magnetic semiconductors as well as spin-glasses

Primary author: Prof. ERIKSSON, Olle (Uppsala University)

Presenter: Prof. ERIKSSON, Olle (Uppsala University)

Contribution ID: **271** Type: **not specified**

The role of higher multipoles in magnetically ordered systems

Wednesday, February 24, 2010 2:15 PM (1 hour)

In most magnetic phase transitions the focus is on the lowest multipole, the dipole which is directly related to the magnetic moment. We will in this work argue that in some cases higher order multipoles are driving the transition and the dipole is a secondary effect.

The concept of spherical tensors or multipoles of an open atomic shell is first reviewed and discussed.Some of these multipoles play an important rule in e.g. x-ray circular dichroism measurements, where with the use of the famous sum rules by Carra et al. the spin and orbital magnetic moments can be deduced.

Then we will describe how such multipoles can be calculated in general in both the ground state as well as excited states in terms of density functional methods including a local correlation term, as in e.g. the so-called LDA+U or LDA+DMFT methods. It will be demonstrated how these multipoles can contribute significantly to the exchange and correlation energies of transition metal systems.

Especially, we will discuss in some depth materials where these multipoles act as the main order parameter, sometimes referred to as an “hidden order”. Especially, results for two cases will be presented the magnetic/superconducting iron-pnictide LaOFeAs and the heavy fermion compound URu2Si2.

Primary author: Dr NORDSTRÖM, Lars (Uppsala University)

Presenter: Dr NORDSTRÖM, Lars (Uppsala University)

Contribution ID: **272** Type: **not specified**

Infulence of the range of interaction in thin magnetic structures

Thursday, February 25, 2010 10:15 AM (1 hour)

The properties of ultrathin magnetic structures are influenced by many length scales that reflect both generic physics and chemical detail. A striking example is the experimentally determined shift of the critical temperature as a function of film thickness. While all systems experience a pronounced suppression in Tc with decreasing film thickness, the magnitude of this shift cannot be reconciled with established theoretical results. In particular, the ratio between the monolayer and bulk limits for the nearest neighbour Ising model is roughly 1/2, whereas experimentally, ratios of the order of 0.1 are commonly measured. By means of detailed Monte Carlo simulations, we resolve this discrepancy by investigating a model with long-range interactions. The model also captures other features of real ultrathin magnets, such as an almost linear temperature dependence for the surface magnetization. Our results demonstrate that the behavior of ultrathin magnetic structures arises from a competition of length scales dictated by their slab-like geometry, the presence of surface boundaries, and crucially, the range of the interactions present.

Primary author: TARONI, Andrea (Uppsala University)

Presenter: TARONI, Andrea (Uppsala University)

Contribution ID: **273** Type: **not specified**

Software Development

Thursday, February 25, 2010 1:15 PM (2 hours)

Open forum

Contribution ID: **274** Type: **not specified**

Magnetic scattering from structured surfaces

Friday, February 26, 2010 10:15 AM (1 hour)

Primary author: Dr HASE, Tom (University of Warwick)

Presenter: Dr HASE, Tom (University of Warwick)

Contribution ID: **275** Type: **not specified**

Discussions and Future Perspectives

Friday, February 26, 2010 11:15 AM (1 hour)

Primary author: Prof. HJÖRVARSSON, Björgvin (Uppsala University)

Presenter: Prof. HJÖRVARSSON, Björgvin (Uppsala University)

Contribution ID: **276** Type: **not specified**

Discussion

Friday, February 19, 2010 11:15 AM (45 minutes)

Contribution ID: **277** Type: **not specified**

Discussion

Friday, February 19, 2010 2:15 PM (45 minutes)