ESS Symposium on Spin Dynamics

Abingdon, 23–24 February, 2012

ESS Symposium on Spin Dynamics — Invited Talks

Thursday 23 February, 2012

11.00 Alan Tennant (Helmholtz-Zentrum Berlin)

Thermal effects in quantum magnets

11.18 Christian Rüegg (Paul Scherrer Institut)

Neutron spectroscopy studies of low-dimensional spin systems

Quantum spin systems offer a wealth of opportunities to discover and investigate the exotic ground states and excitations hidden in magnetic matter. Neutron scattering plays a key role in this area of research. Developments in instrumentation (e.g. ToF spectroscopy at ISIS) and sample environment (magnetic fields, pressure and low temperatures) enable unparalleled studies of spin correlations in these systems. Recent results from a number of prototypical low-dimensional model materials, including chain, ladder and frustrated systems, will be presented and discussed with special focus on future challenges in instrumentation and science at ESS.

11.36 Henrik Rønnow (EPFL)

Breaking the Waves

The spin wave approximation is our workhorse to describe dynamics in magnetically ordered systems. We discuss how inelastic neutron scattering experiments can address the departure from simple spin-wave excitations fit emphasis on the two-dimensional square lattice.

11.54 Tom Fennell (Paul Scherrer Institut)

Power-law spin correlations and dynamics in the spin liquid $Tb_2Ti_2O_7$

The rare earth titanate $Tb_2Ti_2O_7$ is usually described as a spin liquid with very short-range spin correlations and spin fluctuations persisting to 0.05 K. Using a combination of polarized diffuse scattering and triple axis spectroscopy measurements, we show instead that the spin correlations in the low temperature state have a power-law form. Investigations of the spin dynamics using TOF spectroscopy combined with polarized-TAS will also be discussed.

12.12 Radu Coldea (Oxford)

Spin dynamics in the frustrated honeycomb antiferromagnet Na_2IrO_3

We explore the spin dynamics in the frustrated honeycomb antiferromagnet Na_2IrO_3, a candidate to display novel ground states stabilized by the strong relativistic spin-orbit coupling at the $5d$ Ir ions. In powder inelastic neutron scattering at ISIS and ILL using an optimised setup to minimise neutron absorption by Ir we observe evidence for dispersive spin wave excitations of the Ir moments below a zone-boundary energy of 5 meV. The observed dispersion can be quantitatively accounted for by including frustrated in-plane exchanges up to 3rd neighbour, which we propose stabilize zig-zag antiferromagnetic order on the honeycomb lattice.

14.00 Elizabeth Blackburn (Birmingham)

Spin dynamics as a probe of underlying magnetic structures

We can find out a lot of information about a magnetic structure and its physical properties by looking at the magnetisation dynamics. This applies to complicated non-collinear magnetic structures directly, but is also very relevant to, for example, iron-based superconductors (e.g. exchange constant studies), and unconventional superconductors where magnetic order and superconductivity coexist. I will look at some current work in this area, relating primarily to complicated magnetic structures in correlated electron systems, and then look to the future, and what demands this may make on instrumentation and sample environment.

14.18 Phillipe Bourges (Laboratoire Léon Brillouin, CEA Saclay)

Ising-like magnetic excitations in a single-layer cuprate superconductor

The phase diagram of the high-temperature cuprate superconductors is characterized by the pseudogap phenomenon, a set of anomalous physical properties below the characteristic temperature T^* but above the superconducting transition temperature T_c. Recent polarized neutron diffraction experiments demonstrated the universal existence of an unusual magnetic order below T^* showing that the pseudogap regime constitutes a genuine new phase of matter rather than a mere crossover phenomenon. Later on, two excitations associated with the unusual order were observed in $HgBa_2CuO_{4+d}$, suggesting a particular type of order involving circulating orbital currents. Their intensities rise below the same temperature T^* and their dispersions are weak, as expected for an Ising-like order parameter.

14.36 Markus Braden (Cologne)

Magnetic excitations in the pure iron arsenides $BaFe_2As_2$ and LiFeAs

Magnetic correlations in LiFeAs and in $BaFe_2As_2$ were analysed using polarized and unpolarized neutron scattering techniques. The anisotropy of the magnetic excitations in $BaFe_2As_2$ was studied with polarization analysis which allows one to separate the components of the magnetic response. In view of the in-plane ordered moment one might expect easy-plane anisotropy. We find, however, the in-plane polarized magnon to lie at higher energy than the out-of-plane polarized ones indicating very strong in-plane single-ion anisotropy. This finding corroborates the strong electronic signatures of this — structurally only weakly distorted — orthorhombic phase. Superconducting LiFeAs was analyzed concerning the local spin susceptibility and its inelastic magnetic response. We find the suppression of local susceptibility expected for spin-singlet pairing. Inelastic correlations appear at the incommensurate wave vector $(0.5 \pm \delta, -0.5 \pm \delta, 0)$ with $\delta \sim 0.07$ slightly shifted from the commensurate ordering observed in other FeAs-based compounds. The incommensurate magnetic excitations respond to the opening of the superconducting gap by a transfer of spectral weight.

14.54 Andrew Huxley (Edinburgh)

15.12 Dmytro Inosov (MPI Stuttgart)

Itinerant spin dynamics in iron-selenide superconductors

We employ inelastic neutron scattering to study the reciprocal-space structure and dispersion of magnetic excitations in the normal and superconducting states of single-crystalline $A_{1-x}Fe_{2-y}Se_2$ (A =K, Rb). We show that the magnetic resonant mode in these compounds has a quasi-two-dimensional character, similar to overdoped iron-pnictide superconductors. Moreover, it has a rich in-plane structure that is dominated by four elliptical peaks, symmetrically surrounding the Brillouin zone corner, without $\sqrt{5} \times \sqrt{5}$ reconstruction. We also present evidence for the dispersion of the resonance peak, as its position in momentum space depends on energy. Comparison of our findings with the results of band structure calculations provides strong support for the itinerant origin of the observed signal. It can be traced back to the nesting of electron-like Fermi pockets in the doped metallic phase of the sample in the absence of iron-vacancy ordering.

16.30 Giacomo Ghiringhelli (Milan)

Spin excitations in high T_c superconductors studied by resonant inelastic x-ray scattering

When working at the $L_{2,3}$ absorption edges of $3d$ transition metals, resonant inelastic x-ray scattering (RIXS) provides an element and site selective access to electronic and spin related excitations. The large absorption cross sections allow working on thin films and very small samples too, which is not the case for neutron scattering. I will introduce the technique and present results on undoped and doped cuprates. Data show that the magnetic spectral weight is preserved in doped compounds over most of the first Brillouin zone, thus strengthening the importance of spin excitations in the context of HTS.

16.48 Jon Goff (Royal Holloway University of London)

Spin correlations in the paramagnetic phase

Exchange interactions in magnetic systems are usually determined via the excitations from the ordered phase using single-crystal inelastic neutron scattering. Studies of spin correlations in the paramagnetic phase often provide a useful complement to this information. These measurements of weak diffuse magnetic scattering from low-spin quantum systems using polarised neutrons are currently extremely challenging. However, the high flux at ESS could potentially revolutionise this field. I shall illustrate this using a quantum solid, a model magnet, a high-T_c superconductor and a system where spin and orbital degrees of freedom interact.

17.06 Raymond Osborn (Argonne National Laboratory)

Neutrons as a Probe of Electronic Structure

Recent developments at pulsed neutron sources promise the most significant advance in neutron spectroscopy since Brockhouse devised the triple-axis spectrometer. Time-of-flight spectrometers are effective probes of coherent excitations but less effective in investigating strongly Q-dependent fluctuations with a broad frequency response. These limitations can be overcome by sweeping the sample orientation to measure four-dimensional $S(\mathbf{Q}, \omega)$. One field where this will have an impact is in comparison with *ab initio* calculations of the dynamic susceptibility of electronic excitations in strongly correlated electron systems. I will illustrate this with results on $CePd_3$ and the pnictides.

17.24 Stephane Raymond (CEA Grenoble)

Evolution of the spin resonance of $CeCoIn_5$ as a function of magnetic field and chemical substitution

In many unconventional superconductors, a feedback of superconductivity on the magnetic excitation spectrum manifests as a resonance peak occurring below T_c at an energy $\Omega_{res} \approx 2$–$8\ k_B T_c$. We will present the impurity and magnetic field effects on the spin resonance of the heavy fermion superconductor $CeCoIn_5$ ($T_c = 2.3$ K). For non-magnetic La and magnetic Nd impurities, we found that the ratio $\Omega_{res}/k_B T_c$ is constant in agreement with impurity pair breaking effect for $d_{x^2-y^2}$ superconductor. The study under magnetic field of pure $CeCoIn_5$ points to the anisotropy of the resonance and the Zeeman effect for such a strongly Pauli limited superconductor.

17.42 Jonathan White (Paul Scherrer Institut)

Coupling of ferromagnetism and ferroelectricity by multi-component magnetism in the new multiferroic Mn_2GeO_4

As the number of magnetically-driven multiferroic materials continues to increase, so does both the rich diversity of the observed magnetoelectric phenomena. Here we focus on a study of the new multiferroic (MF) Mn_2GeO_4 (MGO), which exhibits a rich array of static properties stemming from competing magnetic interactions. The MF phase supports spontaneous ferromagnetic and ferroelectric orders, the coupling of which is mediated a single multi-component magnetic structure. The spin-wave dispersion has been studied by INS, thus revealing the temperature-evolution of the excitations underpinning the magnetically-driven MF state. We discuss the prospects that MGO may prove to be a model material for studies of magnetoelectric dynamics.

Friday 24 February, 2012

08.45 Arno Hiess (European Spallation Source)

The European Spallation Source

I will give an update on the ESS project, with particular reference to instrumentation for neutron spectroscopy.

09.15 Jörg Voigt (Jülich Centre for Neutron Scattering)

Chopper spectrometers for ESS

Direct geometry time of flight spectrometers benefit especially from pulsed spallation sources. It has been shown that in particular instruments using cold neutrons profit strongly from the long pulse at ESS [1,2].

Reviewing recent publications from world class TOF spectrometers shows that often one uses high energy and low energy neutrons for comprehensive studies of the dispersion in novel functional materials. As an example, the excitation spectrum in high temperature superconductors extends well above 200 meV, while interesting features of the spectrum require good resolution and therefore lower energies.

We discuss chopper spectrometers at a long pulse spallation source targeting different applications. The high peak flux allows to achieve the highest energy resolution ranging to the area of backscattering, while using the long pulse an instrument can be tuned to high flux e.g. for kinetic or parametric studies that are limited by the flux of current sources.

[1] K. Lefmann, H. Schober, F. Mezei, Meas. Sci. Techno. 19, 034025 (2008).

[2] H. Schober et al., NIM **A 589**, 34–46 (2008).

09.30 Henrik Rønnow (EPFL)

The Danish–Swiss ESS multi-crystal analyser spectrometer project

14.30 Jeroen van den Brink (IFW Dresden)

Elementary magnetic excitations of iridates and cuprates probed by resonant inelastic X-ray scattering

Resonant Inelastic X-ray Scattering (RIXS) provides direct access to elementary charge, spin and orbital excitations in complex oxides. As a technique it has made tremendous progress with the advent high-brilliance synchrotron X-ray sources. From the theoretical perspective the fundamental question is to which precisely which low-energy correlation functions RIXS is sensitive. Depending on the experimental RIXS setup, the measured charge dynamics can include charge-transfer, phonon, d-d and orbital excitations [1,2]. I will show that RIXS also allows to probe spin dynamics, in particular magnon and bi-magnon dispersions [3,4]. Based on these observations, I will discuss the novelties that RIXS reveals on the spin dynamics of high-T_c cuprates [5,6] and strongly spin-orbit coupled iridium oxides [7].

[1] L. Ament, M. van Veenendaal, T. Devereaux, J.P. Hill and JvdB, Rev. Mod. Phys. **8**3, 705 (2011). [2] F. Forte, L. Ament and JvdB, PRL **101**, 106406 (2008). [3] L. Braicovich et al., PRL **102**, 167401 (2009). [4] L. Ament, G. Ghiringhelli, M. Moretti Sala, L. Braicovich and JvdB, PRL **103**, 117003 (2009). [5] L. Braicovich et al., PRL **104**, 077002 (2010). [6] M. Guarise et al., PRL **105**, 157006 (2010). [7] L. Ament, G. Khaliullin and JvdB, PRB **84**, 020403 (2011).

15.00 Collin Broholm (Johns Hopkins University)

15.30 John Hill (Brookhaven National Laboratory)

X-ray scattering studies of equilibrium and non-equilibrium spin dynamics in strongly correlated systems

In this talk, I will discuss the power of x-rays to probe dynamics in strongly correlated systems. I will first present recent resonant inelastic x-ray scattering measurements of the spin dynamics in a single La_2CuO_4 layer and in a one-dimensional iridate compound, Sr_3CuIrO_6. In the second half of the talk, I present femtosecond elastic scattering measurements of a static, stripe-ordered, non-superconducting cuprate, $La_{1.875}Ba_{0.125}CuO_4$, following ultra-fast excitation with mid-IR phonons. By studying the temporal evolution of the LTT phase and of the charge order one is able to draw conclusions about the competition of each with 3D phase coherent superconductivity.

ESS Symposium on Spin Dynamics — Posters

Thursday 23 February, 15.30–16.30 and 18.30–19.30

Sala Gabriele (Royal Holloway University of London)

Field Trip Inside Spin Ice

We study the distribution of magnetic fields h, inside spin ice. This study reflects the monopolar field set up by defects in a spin ice configuration, and we discuss its manifestations in experiments involving local field probes such as NMR or muon spin rotation. Averaged over the bulk of the sample, this distribution resembles one set up by a random spin arrangement. However, the density of low-field locations decreases as the local ferromagnetic correlations imposed by the ice rules develop. The $1/r^2$ Coulomb field of a single monopole is visible in (magnetic) voids of the lattice where lattice-scale effects due to the immediate proximity of other spins are suppressed.

Arno Hiess (European Spallation Source, Lund)

The microscopic spin dynamics in the normal and superconducting state of UBe_{13}

Neutron spectroscopy has been of importance to appreciate the interrelation of magnetism and superconductivity by revealing the microscopic spin dynamics. We here present experimental results on the cubic correlated 5f superconductor UBe_{13} obtained by high-resolution cold neutron three-axis spectroscopy. The energy dependence of the longitudinally polarized spin dynamics in the normal state can be modeled superimposing a quasi-elastic contribution and an inelastic contribution. In the superconducting state spectral weight shifts to higher energies indicating the opening of a superconducting gap is reflected in the spin dynamics. The shift coincides with the inelastic contribution already present in the normal state.

Mattia Mena (London Centre for Nanotechnology, University College London)

Magnetic structure and excitations of the one-dimensional quantum antiferromagnet $RbCoCl_3$

Here we report the results of an inelastic neutron scattering experiment of the magnetic excitations in $RbCoCl_3$, a quasi-1D Ising-like antiferromagnet, performed on LET (ISIS, RAL). The material undergoes two phase transitions. Between the Neel temperature $T_{N1} = 28$ K and $T_{N2} = 14$ K, as well as above T_{N1}, pairs of domain-wall excitations characteristic for an Ising magnet are observed. Below T_{N2} an additional splitting of the modes is discovered. Results and preliminary analysis of the data will be presented and discussed.

Dominic Moseley (Imperial College London)

Magnetotransport experiments on an iron-based superconductor

Iron-based superconductors have reinvigorated the superconductivity community by providing a new system to probe superconducting quantum phenomena and the interplay between magnetism and electronic transport. To elucidate these effects we have performed magnetotransport experiments as a function of field and temperature on single crystals of the archetypal

iron-based superconductor, $BaFe_2As_2$. Our findings show a linear MR above a temperature dependent critical magnetic field, in agreement with previous studies. Currently, the only explanation for this phenomenon is the existence of 'Dirac Cones'— a linear relationship between momentum and energy — which have been theoretically predicted and recently experimentally observed using ARPES techniques.

Joe Paddison (University of Oxford & ISIS Facility)

Magnetic frustration in β-$Mn_{0.8}Co_{0.2}$ and MnO

I present an analysis of spin correlations in the paramagnetic phases of β-$Mn_{0.8}Co_{0.2}$ and MnO — two systems in which frustration of magnetic interactions plays a key role. New neutron data shows that β-$Mn_{0.8}Co_{0.2}$ remains magnetically disordered to 50 mK. I look at possible explanations for this unusual behaviour, using reverse Monte Carlo and mean-field techniques to fit our data. We have also been able to fit a large volume of magnetic diffuse scattering for MnO at 160 K, and I give an analysis of the spin correlations in terms of the frustration of the crystal lattice.

Attila Szilva (University of Uppsala)

Magnetic interactions in correlated systems

We present a general approach for calculating magnetic exchange parameters from first-principles. The strategy of the determination of the generalized Heisenberg exchange parameters and Dzyialoshinski–Moriya vector is to use the so-called local force theory. The noncollinear-relativistic exchanges formulas are given in terms of a real-space LMTO-ASA scheme. The corresponding torque and effective Hamiltonian expressions in correlated systems are also determined using a spin-polarized bare Green function.

Bruno Tomasello (University of Kent & ISIS Facility)

characteristic time-scales in spin ice

The Emergence of magnetic monopoles in Spin Ice materials attracts lot of interest from the scientific community. Not only for its singular properties that displays novel physical phenomena, but also for their possible implementation in new technologies. A description for the dynamics of such monopoles is then of crucial importance. The hopping of a magnetic monopole in Spin Ice from one site to the next, consists of the flip of a large spin from an easy axis configuration to the opposite one. Here we investigate the role that quantum-mechanics play when a spin flips from one configuration to the other. We focus, in particular, on time-evolution starting from some given initial conditions, proposing an estimation for the characteristic time-scales detectable in this system.

Linda Udby (University of Copenhagen)

Magnetic order in high-T_c Sr/O co-doped $La_{2-x}Sr_xCuO_{4+y}$

We present results of magnetic elastic neutron scattering experiments on the co-doped superoxygenated $La_{2-x}Sr_xCuO_{4+y}$ system with $x = 0.04$, 0.065 and 0.09. The spin-density wave has been studied and we find incommensurate antiferromagnetic order below T_N coinciding with the superconducting ordering temperature $T_c = 40$ K for all dopings. The incommensurability

value is consistent with a hole-doping of $n_{\mathrm{h}} \geq 1/8$ and the magnetic order is correlated over long distances, however decreasingly so with increasing Sr content.

Mehran VafaeeKhanjani (Technical University of Darmstadt)

Magnetic and electrical properties of the possibly antiferromagnetic half-metal double perovskite La_2CrWO_6

The combination of a magnetic ion (B-site) and a non-magnetic ion (B'-site) in double perovskites ($A_2BB'\mathrm{O}_6$) can lead to an induced magnetic moment at the non-magnetic site. Therefore, double perovskites are hot candidates in the search for compensated antiferromagnetic half-metals (AFM-HMs) which are considered to be useful for spintronics, supplying on the one hand, fully spin-polarized electrons, and on the other hand due to the antiferromagnetic configuration, they are magnetically stable. Following band structure calculations and a simple ionic picture, $\mathrm{La_2CrWO_6}$ is an AFM-HM candidate. However, as bulk material this compound is thermodynamically unstable. One way of synthesizing such a material is a thin film approach forcing W into a very unusual $\mathrm{W^{3+}}$ state. To our knowledge, we have synthesized for the first time $\mathrm{La_2CrWO_6}$ by pulsed laser deposition. Crystal structure, magnetic and electrical properties are presented.

Simon Ward (Paul Scherrer Institut & University College London)

Effects of bond disorder in the quantum spin ladder $(C_5H_{12}N)_2CuBr_{4(1-x)}Cl_{4x}$

There has been a resurgence of interest in low-dimensional spin systems, driven by the discovery of new model materials. One such class of materials are spin ladders for which $(\mathrm{C_5H_{12}N})_2\mathrm{CuBr_4}$ is an exceptional realisation with exchange interactions $J_{\mathrm{rung}} = 12.8$ K, $J_{\mathrm{leg}} = 3.4$ K. Here we present new inelastic neutron scattering results on the related spin ladder materials $(\mathrm{C_5H_{12}N})_2\mathrm{CuCl_4}$ and $(\mathrm{C_5H_{12}N})_2\mathrm{CuBr}_{4(1-x)}\mathrm{Cl}_{4x}$ with $x = 0.1$. In the pure Cl compound exchange parameters are reduced to $J_{\mathrm{rung}} = 3.4$ K, $J_{\mathrm{leg}} = 1.3$ K. In the Br rich compound the effect of disorder is clearly manifest in the spectral function of the triplet modes with a renormalised spin gap and a finite life time.