MA 15: Spin structures and Magnetic Phase Transitions

Time: Tuesday 9:30–13:15 Location: HSZ 403

MA 15.1 Tue 9:30 HSZ 403

The prototype chiral ferromagnet FeGe: phase diagram, Skyrmions and ^{57}Fe magnetic resonance — •Michael Baenitz[1], Panchanan Khuntia[1], Markus Schmidt[1], Ulrich Roessler[2], and Heribert Wilhelm[3] — [1]MPI for the Chemical Physics of Solids, 01187Dresden, Germany — [2]Leibniz Institute for SolidState and Materials Research, 01171 Dresden, Germany — [3]Diamond Light Source Ltd, Didcot, Oxfordshire,United Kingdom

The helical ferromagnet FeGe belongs to the class of B20 compounds with non-centrosymmetric structure being essential for new forms of ferromagnetic phases (confined or modulated Skyrmion phases). From an NMR point FeGe is a prototype system to study chiral excitations directly "on-site" via the ^{57}Fe nucleus because of its S=1/2 nuclear spin. Here, in contrast to MnSi or MnGe (where ^{55}Mn has S=5/2), the absence of quadrupolar interactions, which usually creates broad NMR lines, makes detailed investigations of the anisotropic Zeeman interaction in internal/external fields possible. ^{57}Fe NMR allows to probe the local susceptibility (hyperfine field), the dynamic susceptibility (spin lattice relaxation rate) and the spin-spin interaction directly "on site". Additionally the NMR line itself (its Fourier transform) provides information about the multiplicity of the Fe sites in the complex helimagnet. ^{57}Fe NMR was performed on crushed single crystals of ^{57}Fe enriched FeGe material between 2-300 K in zero and applied magnetic fields. Phase boundaries in the ordered state are identified and critical dynamics in the vicinity of these boundaries are obtained from the spin-lattice and spin-spin relaxation rate.

MA 15.2 Tue 9:45 HSZ 403

Fluctuation-induced First Order Quantum Phase Transition of U(1) Quantum Spin Liquid in Pyrochlore Quantum Antiferromagnet — •Imam Makhfudz — Johns Hopkins University, Baltimore, USA

We predict using quantum free energy calculation that the quantum phase transition between U(1) quantum spin liquid (QSL) and antiferromagnet (AFM) phases in pyrochlore quantum antiferromagnet (QAFM) is a first order rather than second order. This change in order from second to first order is induced by gauge fluctuations, which are explicitly taken into account at gauge theory level in our effective low energy theory. We therefore have discovered a fluctuation-induced first order quantum phase transition in pyrochlore QAFM. We explicitly derive the quantum free energy description of this QSL to AFM phase transition and predict that it is a weakly first order phase transition. We also briefly discuss the experimental relevance of this result.

MA 15.3 Tue 10:00 HSZ 403

Investigation of the Spin-Peierls Transition in $TiPO_4$ — •Patrick Reuvekamp[1], Reinhard K. Kremer[1], Joseph M. Law[2], and Robert Glaum[3] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Rheinische Friedrich-Wilhelms-Universität, Institut für Anorganische Chemie, Bonn, Germany

At room temperature, $TiPO_4$ crystallizes in the orthorhombic $CrVO_4$ structure type characterized by one-dimensional equidistant Ti atoms running along the $\boldsymbol{c}$-axis. From high temperature magnetic susceptibility measurements, the afm intrachain spin exchange between the Ti^{3+} ($3d^1$, $S = 1/2$) cations was observed to be 965 K which is remarkably large for a spin-Peierls (SP) compound.[1] Below room temperature, a two stage SP transition occurs comprising two sequential magnetostructural phase transitions at $T_{c2} \sim 110$ K and $T_{c1} \sim 74$ K into a non-magnetic singlet groundstate. NMR measurements indicated the intermediate phase to be incommensurate.[1] Utilizing low-temperature single-crystal x-ray diffraction and thermal expansion measurements, we investigated in detail the temperature and magnetic field dependence of these two transitions and observed a dimerization of the Ti chains below T_{c2}. We observed that only the T_{c1} transition is dependent on the magnetic field. At 9 T, T_{c2} decreases by ~ -100 mK. The magnetic field dependence of $\Delta T_{c1}/T_{c1} \propto H^2$, consistent with standard SP theory.[1]J. M. Law *et al.*, Phys. Rev. B **83**, 180414 (2011). [2]M. Bykov *et al.*, Phys. Rev. B **88**, 184420 (2013).

MA 15.4 Tue 10:15 HSZ 403

Magnetic transitions in Mn/Ag(111) — •Jingfan Ye, Franziska Lambrecht, Timofey Balashov, and Wulf Wulfhekel — Physikalisches Institut, Karlsruhe Institute of Technology, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany

An antiferromagnetic manganese monolayer on Ag(111) exhibits a 120°-Néel structure due to geometric frustration [1]. Using a spin-polarized scanning tunneling microscope, we investigated the ground state of Mn islands on Ag(111) of sizes between 10 and 10000 nm^2 at 4K. We found out that the magnetic contrast disappears below a certain island size. In an intermediate region, it was also possible to observe switching between different configurations of the Néel state, at a rate scaling linearly with an externally applied magnetic field. We attribute the observed effects to a quantum phase transition, in which the anisotropy barrier between the classical ground states is lowered with decreasing island size and increasing magnetic field [2].

[1] C.-L. Gao et al. *Phys. Rev. Lett.* **101**, 267205 (2008)
[2] P. Legett et al. *Rev. Mod. Phys.* **59**, 1-85 (1987)

MA 15.5 Tue 10:30 HSZ 403

Spin structures and electron lattice coupling in the double perovskite Sr_2FeOsO_6 — Avijit Kumar Paul[1], •Peter Adler[1], Manfred Reehuis[2], Vadim Ksenofontov[3], Binghai Yan[1], Martin Jansen[1], and Claudia Felser[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany — [3]Johannes Gutenberg-Universität, Mainz, Germany

Double perovskites with an ordered arrangement of transition metal $3d$ and $4d$ or $5d$ sites show remarkable magnetic properties like half-metallic ferromagnetism below 400 K in Sr_2FeMoO_6 or ferrimagnetism with a high T_C of 725 K in the insulator Sr_2CrOsO_6. We have studied the magnetic and electronic properties of insulating Sr_2FeOsO_6 by neutron powder diffraction, ^{57}Fe Mössbauer spectroscopy and spin-polarized density functional theory calculations. Sr_2FeOsO_6 shows two magnetic phase transitions below 140 and 67 K, respectively. Similar as in related systems the spin structures reveal ferrimagnetic ordering of Fe and Os moments within the planes of the tetragonal crystal structure. Along c, however, two different spin alignment patterns are adopted which lead to overall antiferromagnetic behavior. Our experimental and theoretical results suggest a frustrated magnetic behavior, where the frustration is partially released by a Peierls-like lattice modulation and a switch of the spin structure below 67 K. Thus, Sr_2FeOsO_6 features an intimate interplay of lattice, spin and orbital degrees of freedom.

MA 15.6 Tue 10:45 HSZ 403

Absorption and photoluminescence spectroscopy on copper metaborate CuB_2O_4 — •Dennis Kudlacik[1], J. Debus[1], R. V. Pisarev[2], D. Dunker[1], D. R. Yakovlev[1,2], and M. Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

CuB_2O_4 contains two nonequivalent Cu^{2+} sublattices, each with different magnetic ordering. The magnetic structure is dominated by the antiferromagnetic order of the 4b sublattice. Interactions may transfer it to the 8d sublattice where it shall coexist with a paramagnetic component. Three different magnetic phase transitions can be observed below 21 K.[1] Accordingly, it is an ideal candidate to probe magnetic interactions between both sublattices as a function of temperature and, for example, optical excitation. We have studied linear-polarized absorption spectra, magneto-photoluminescence (PL) and photoluminescence excitation (PLE) of CuB_2O_4. The absorption and PL spectra show a rich fine structure containing up to six zero phonon lines. We compare the intensities of the zero phonon lines and magnon related emission lines for the different states of magnetic ordering. Also, the PLE spectroscopy reveals the coupling between the 8d and 4b sublattices. On the whole, the applied optical techniques grant access to crystallographic and magnetic properties of CuB_2O_4.

[1] R.V. Pisarev et al., Phys. Rev. Lett. 93, 037204 (2004).

MA 15.7 Tue 11:00 HSZ 403

Spin relaxation in frustrated 2D antiferromagnets α-ACr_2O_4 (A = Ca, Sr) — •Martina Schädler, Mamoun Hemmida, Hans-Albrecht Krug von Nidda, and Alois Loidl — Experimental

Physics V, EKM, University of Augsburg, 86135 Augsburg, Germany

Electron Spin Resonance (ESR) measurements were performed at X-band (9.4 GHz) and Q-band (34 GHz) frequency on polycrystalline samples of α-$CaCr_2O_4$ and α-$SrCr_2O_4$. In both compounds the magnetic Cr^{3+} ions form slightly distorted triangular layers, representing a frustrated 2D Heisenberg antiferromagnet with alternating exchange. The spin-spin relaxation behavior derived from the temperature dependence of the ESR-linewidth (ΔH) exhibits two different regimes. At temperatures $T > 2T_N$ a BKT-like scenario [1,2] suggests the existence of Z_2 vortices as observed in the prototype triangular lattice Heisenberg antiferromagnet $CuCrO_2$ [3]. For $T_N < T < 2T_N$ fluctuations due to the onset of 3D antiferromagnetic order seem to dominate.

We thank for sample preparation: S. Toth and B. Lake, Helmholtz Zentrum Berlin, Germany (α-$CaCr_2O_4$), S. E. Dutton and R. J. Cava, Princeton University, USA (α-$SrCr_2O_4$).

References: [1] V. L. Berezinskii, J. Exp. Theor. Phys. **32**, 493 (1971). [2] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973). [3] M. Hemmida, H.-A. Krug von Nidda, and A. Loidl, J. Phys. Soc. Jpn. **80**, 053707 (2011).

15 min. break

MA 15.8 Tue 11:30 HSZ 403

Restoration of 2D Ising criticality in dipolar-frustrated ferromagnetic films — •Danilo Andrea Zanin[1], Niculin Saratz[1], Boris Sangiorgio[1], Thomas C.T. Michaels[2], Alessandro Vindigni[1], Urs Ramsperger[1], and Danilo Pescia[1] — [1]ETH Zurich, Switzerland — [2]University of Cambridge, United Kingdom

For about three decades the quest for novel paradigms for magnetostorage and spintronics has driven the development and investigation of magnetic nanostructured materials. For instance, the study of films magnetized in plane led to the observation of the two-dimensional Ising critical behavior. In films with easy axis directed out of plane the magnetization spontaneously splits into domains because of the competition between short-range exchange coupling and long-range dipolar interaction. A shrinking of the magnetic domains of in these films with increasing temperature was already observed, e.g., in Fe/Cu(001) samples by means of Scanning-Electron-Microscopy with Polarization Analysis (SEMPA). This phenomenon drives the occurrence of reentrant transitions of magnetic-domain patterns. However, approaching the Curie temperature, magnetic domains become mobile within the timescale of the experiment, which consequently blurs the SEMPA images. In order to extend the phase diagram to higher temperatures, we performed Magneto-Optic Kerr Effect (MOKE) experiments. Even though our MOKE setup does not allow a direct visualization of micrometric magnetic domains, by means of statistical analysis of the large data set, we identify clearly the transition between uniform to domain phase as a function of temperatures and applied magnetic field.

MA 15.9 Tue 11:45 HSZ 403

Quantifying entanglement with scattering experiments — •Oliver Marty[1], Michael Epping[2], Hermann Kampermann[2], Dagmar Bruss[2], Martin Plenio[1], and Marcus Cramer[1] — [1]Institut für Theoretische Physik, Universität Ulm — [2]Institut für Theoretische Physik III, Heinrich-Heine-Universität Düsseldorf

We show how the entanglement contained in states of spins arranged on a lattice may be quantified with observables arising in scattering experiments. We focus on the partial differential cross-section obtained in neutron scattering from magnetic materials but our results are sufficiently general such that they may also be applied to, e.g., optical Bragg scattering from ultracold atoms in optical lattices or from ion chains. We discuss resonating valence bond states and ground and thermal states of experimentally relevant models–such as Heisenberg, Majumdar-Ghosh, and XY model–in different geometries and with different spin numbers. As a by-product, we find that for the one-dimensional XY model in a transverse field such measurements reveal factorization and the quantum phase transition at zero temperature.

[1] O. Marty et al., arXiv:1310.0929

MA 15.10 Tue 12:00 HSZ 403

Chiral spin liquid in a two-dimensional two-component helical magnet — •Olga Dimitrova — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany

A low-temperature method is developed, suited for a two-dimensional two-component classical helical magnet. Four phases on the phase diagram as functions of the temperature and the helicity parameter of the Hamiltonian are found. Among the three ordered phases two show magnetic order: the usual algebraic correlations of the magnetization and the algebraic correlations of the magnetization in the frame rotating according with the helical order. A chiral spin liquid phase emerges directly from the paramagnetic phase and has a scalar parity-breaking pitch of the magnetization as the order parameter. The chiral phase transition is found to be of a continuous second order type with a modified by the long-range interaction Ising universality class. All the critical exponents are calculated in the second and the third order of an ϵ-expansion. A new scaling relationship replacing the Josephson's one is found.

MA 15.11 Tue 12:15 HSZ 403

Studying finite-temperature magnetism using relativistic disordered local moment theory — •Andras Deak[1], Eszter Simon[1], Manuel dos Santos Dias[2], Laszlo Szunyogh[1], and Julie B. Staunton[3] — [1]Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [3]Department of Physics, University of Warwick, United Kingdom

Numerical investigations of magnetic phenomena at finite temperatures are mostly based on Heisenberg-type spin models treated with methods of statistical physics (Monte Carlo or Langevin dynamics simulations). Although the parameters of such models can be obtained from first principles calculations, neglecting higher-order spin interactions and longitudinal spin fluctuations may impose drastic restrictions on the applicability of such approaches.

In this talk we present a "first principles only" approach to studying finite-temperature magnetism. The method is based on the Disordered Local Moment (DLM) picture that can be merged efficiently with the Local Spin-Density Functional Approximation (LSDA) of Density Functional Theory (DFT). In particular, solving the Kohn–Sham–Dirac equation allows for investigating relativistic effects. We demonstrate the new computational scheme for the temperature dependence of the magnetocrystalline anisotropy energy of chemically ordered and disordered bulk FePt alloys, and the metamagnetic phase transition in bulk FeRh from antiferromagnetic to ferromagnetic phase.

MA 15.12 Tue 12:30 HSZ 403

Evidence of spin-charge correlation and its interplay with superconductivity in 1/8-doped $La_{2-x}Sr_xCuO_4$ and $La_{2-x}Ba_xCuO_4$ – a ^{139}La spin-lattice relaxation study — •Seung-Ho Baek[1], Markus Hücker[2], Andreas Erb[3], Genda Gu[2], Bernd Büchner[1], and Hans-Joachim Grafe[1] — [1]IFW-Dresden, Institute for Solid State Research, PF 270116, 01171 Dresden, Germany — [2]Brookhaven National Laboratory, Upton, New York 11973, USA — [3]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meißner-Straße 8, D-85748 Garching, Germany

We discuss the ^{139}La nuclear magnetic resonance (NMR) spin-lattice relaxation rate T_1^{-1} of $La_{2-x}Sr_xCuO_4$ (LSCO:x, $0.07 \leq x \leq 0.15$) as well as 1/8-doped $La_{2-x}Ba_xCuO_4$ (LBCO:1/8) single crystals. A doping of 1/8-holes induces an unusual spin freezing behavior which, though much weaker, resembles stripe-ordered LBCO:1/8. Together with previous ^{139}La T_1^{-1} data of $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$ (LESCO), we provide compelling evidence that charge order is closely connected with spin freezing occurring in $\sim$ 1/8-doped La cuprates. The unconventional external field dependence of the spin freezing in LSCO:1/8, which is absent in non-superconducting LESCO:0.13 and LBCO:1/8, suggests a competing relationship between charge order and superconductivity.

MA 15.13 Tue 12:45 HSZ 403

RKKY Interactions in Quasiperiodic Systems — •Stefanie Thiem and John Chalker — Theoretical Physics, Oxford University, 1 Keble Road, Oxford OX1 3NP, UK

We study the structure of the magnetic ground state and the low-temperature behaviour of the magnetic moments in quasiperiodic tilings due to the RKKY mechanism. We compute the exchange interactions between the magnetic impurities by a continued fraction expansion of the Green's function of the conduction electrons. Based on these results we apply Monte Carlo simulations to study the alignment of the Ising spins in these tilings.

MA 15.14 Tue 13:00 HSZ 403

Long range magnetic ordering and spin dynamics in

the itinerant magnets $V_{1-x}Cr_xPtGe$ (x=0...0.2) — Sarah Ackerbauer[1], •Helge Rosner[1], Andreas Leithe-Jasper[1], Pabitra Biswas[2], Rustem Khasanov[2], and Yuri Grin[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden — [2]Paul Scherrer Institut, CH-5232 Villigen, Switzerland

Weak itinerant magnets are in the focus of present-day physical studies due to a range of unusual properties, including strong magneto-elastic effects and superconductivity. Despite the large interest in these systems, their theoretical description is far from being fully established. Especially, the interplay or competition of localized moments and band magnetism is only poorly understood. This renders systems composed of usually nonmagnetic elements very suitable for a systematic study of this interplay. Here, we present a joint experimental and theoretical study of the electronic and magnetic properties of the novel compounds $V_{1-x}Cr_xPtGe$ ($x = 0...0.2$). For $x = 0$ the system exhibits strong spin fluctuations, but does not show long range magnetic order down to 2K. Density functional band structure calculations predict the stabilization of a magnetic ground state by moderate electron doping. We realized this experimentally by Cr substitution on the V site and indicate the development of bulk long range magnetic order with T_N up to 15 K by thermodynamic measurements and μ_{SR} measurements.