MA 37: Frustrated Magnets - Strong Spin-Orbit Coupling 2 (joint session TT/MA)

Time: Wednesday 15:00–17:45 Location: HSZ 304

MA 37.1 Wed 15:00 HSZ 304

Magnetic frustration in fcc lattices — •Veronika Fritsch[1], Christina Baumeister[1], F. Maximilian Wolf[1], Johanna Oefele[1], Jens-Uwe Hoffmann[2], Manfred Reehuis[2], and Oliver Stockert[3] — [1]EP 6, Electronic Correlations and Magnetism, Augsburg University, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

A face-centered cubic (fcc) lattice is inherently prone to magnetic frustration, since it is build from a network of edge-sharing tetrahedra. Up to now most studies were performed on insulating systems. We have investigated various metallic systems with neutron diffraction experiments, where the magnetic Ho-ions form an fcc lattice: $HoInCu_4$ and $HoCdCu_4$ [1] as well as $HoInAg_2$ and $HoInAu_2$. All compounds exhibit long-range magnetic order with different propagation vectors, which can be understood within a simple J_1/J_2 model [2]. Furthermore we found diffuse scattering dependent on the degree of frustration of the samples.

[1] V. Fritsch *et al.*, arXiv:1907.09885 [cond-mat.str-el]
[2] P. W. Anderson, Phys. Rev. **79**, 705 (1950).

MA 37.2 Wed 15:15 HSZ 304

The evolution of magnetic frustration in $HoInAg_{2-x}Au_x$ — •Johanna Oefele[1], Oliver Stockert[2], Philipp Gegenwart[1], and Veronika Fritsch[1] — [1]EP6, Electronic Correlations and Magnetism, Augsburg University, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

While the intermetallic compounds $HoInAg_2$ and $HoInAu_2$ share the same face-centered cubic crystal structure and are isoelectronic, the magnetic properties significantly deviate from each other. $HoInAg_2$ is strongly frustrated as evidenced by its thermodynamic properties and a large frustration parameter. In contrast the $HoInAu_2$ system shows no signs of magnetic frustration. In order to explore the transition from the frustrated to the non-frustrated system we synthesised the substitution series $HoInAg_{2-x}Au_x$.

In this talk I will present the crystal growth and the susceptibility, specific heat and the resistivity measurements on our polycrystalline samples. The effective paramagnetic moments extracted from the magnetic susceptibility coincide with the value expected for free Ho^{3+}. From the specific heat the entropy was calculated confirming the presence of magnetic frustration in $HoInAg_2$. With increasing substitution of Ag with Au the Néel temperature is monotonically increasing, while the frustration vanishes.

MA 37.3 Wed 15:30 HSZ 304

Short range spin ice type correlations of Kagome spin ice HoAgGe by diffuse neutron scattering — •Kan Zhao and Philipp Gegenwart — Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Spin ices are exotic phases of matter characterized by frustrated spins obeying local ice rules that minimize the number of spatially isolated magnetic monopoles, in analogy with the electric dipoles in water ice. In two dimensions, one can similarly define ice rules for in-plane Ising-like spins arranged on a kagome lattice, which require each triangle plaquette to have a single monopole, and can lead to a variety of unique orders and excitations.

With P-62m structure, Ho sites of HoAgGe in the ab plane form a distorted kagome lattice. According to magnetometry, thermodynamic measurements, elastic neutron scattering and Monte Carlo simulations, we establish HoAgGe as the unique crystalline system to realize the kagome spin ice state [1].

The short range spin ice type correlations, have been predicted as one characteristic feature of classical kagome spin ice model. Thus, we conducted the diffuse scattering for HoAgGe above the long range magnetic order temperature. And clear diffuse scattering pattern is obtained, which is consistent with that of Monte Carlo simulations based on a classical spin model consisting of Ising-like in-plane spins on the 2D distorted kagome lattice of HoAgGe [1].

[1] Zhao, Kan et al. Submitted (2018)

MA 37.4 Wed 15:45 HSZ 304

New phases in the Shastry-Sutherland compound NdB_4 discovered by high-resolution dilatometry — •Rahel Ohlendorf[1], Sven Spachmann[1], Daniel Brunt[2], Oleg Petrenko[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Department of Physics, University of Warwick, UK

We report detailed thermal expansion and magnetostriction studies on NdB_4 single crystals in magnetic fields up to 15 T. The system can be mapped on a Shastry-Sutherland model implying magnetically frustrated orthogonal dimers of Nd-moments. Accordingly, a sequence of unusual magnetic phases has been reported [1]. At $B = 0$ T these phases are associated with the evolution of antiferromagnetic (afm) order at $T_1 = 17.2$ K and two incommensurate afm phases at $T_2 = 7.0$ K and $T_3 = 4.8$ K. All transitions are associated with pronounced anomalies in the thermal expansion coefficients which enables studying the phase boundaries in external magnetic fields, here applied along the crystallographic [001]- and [110]-axis, respectively. Our data confirm previously reported phase boundaries and show, e.g., that the nature of the phase transition $T_2(B)$ changes from continuous to discontinuous. In addition, for each field direction our data evidence novel phases not reported before. The phase diagram is discussed based on the anomalies in the thermal expansion and magnetostriction data and the respective uniaxial pressure dependencies.

[1] Ryuta Watanuki et al 2009 J. Phys.: Conf. Ser. 150 042229

15 min. break.

MA 37.5 Wed 16:15 HSZ 304

Energy dynamics in the Kitaev quantum spin liquid at finite temperature and momentum — •Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106, Braunschweig, Germany

The role of finite temperature and momentum in the energy dynamics of the two-dimensional Kitaev spin-model on the honeycomb lattice are studied. Fractionalization of magnetic moments into mobile Majorana matter and a static $\mathbb{Z}_2$ gauge field lead to a continuum of energy density modes comprising two channels. Thermal flux excitations, which act as an emergent disorder, strongly affect the dynamical energy susceptibility. Above the flux proliferation temperature, coherent energy propagation is modified into a quasi hydrodynamic density relaxation, the temperature and momentum dependence of which is analyzed. Results from the low-temperature homogeneous gauge and a mean-field treatment of thermal gauge fluctuations, valid at intermediate and high temperatures are considered.

MA 37.6 Wed 16:30 HSZ 304

Raman spectrum of two particle excitations in the Kitaev-Heisenberg bilayer — •Erik Wagner and Wolfram Brenig — Institute for Theoretical Physics, Technical UniversityBraunschweig, Braunschweig, Germany

We study the Raman response of a honeycomb Kitaev spin-model with (an-)isotropic intralayer exchange $J_{x,y,z}$, coupled by additional interlayer Heisenberg exchange J to form a bilayer. Starting from the limit of decoupled dimers we use a perturbative continuous unitary transformation (pCUT), based on the flow equation method, to perform series expansion on the Hamiltonian and the Raman operator to analyze the spectrum. In particular we consider the groundstate energy and one particle dispersion up to 9th order in $J_{x,y,z}$ as well as the two particle interactions and spectrum up to 8th order. Results for the Raman response as well as (anti-)bound states will be presented versus anisotropy and for various bilayer-stackings.

MA 37.7 Wed 16:45 HSZ 304

Excitonic Magnetism at the intersection of Spin-orbit coupling and crystal-field splitting — Teresa Feldmaier[1], Pascal Strobel[1], Michael Schmid[1,2], Philipp Hansmann[3], and •Maria Daghofer[1] — [1]FMQ, Universität Stuttgart, Germany — [2]IQST, Stuttgart and Ulm, Germany — [3]MPI-CPfS, Dresden, Germany

Excitonic magnetism involving superpositions of singlet and triplet states is expected to arise for two holes in strongly correlated and spin-orbit coupled t_{2g} orbitals. However, uncontested material examples for its realization are rare. Applying the Variational Cluster Approach to the square lattice, we find for weak spin-orbit coupling stripy spin antiferromagnetism combined with stripy orbital order without a crystal field and checkerboard spin antiferromagnetism when crystal field favors the xy orbital. Strong spin-orbit coupling leads to excitonic antiferromagnetism that can coexist with substantial orbital polarization. We then address the specific example of Ca_2RuO_4 using *ab initio* modeling and conclude it to realize excitonic magnetism despite its pronounced orbital polarization.

MA 37.8 Wed 17:00 HSZ 304

Influence of spin-orbit coupling onto thermodynamic and dynamic properties of d^5- and d^4-systems — •Jan Lotze and Maria Daghofer — University of Stuttgart, Functional Matter and Quantum Technologies, Pfaffenwaldring 57, 70569 Stuttgart

We investigate the two-dimensional, spin-orbit coupled, three-band Hubbard model in the d^5 and d^4 configuration at finite temperature by means of the variational cluster approximation. Thermodynamic (magnetization, specific heat) and dynamic (DOS, spectral function) properties are presented. We investigate the influence of cluster size and symmetry on the Néel temperature T_N and on spectra.

We find that the DOS of the d^5-system supports the picture of a system between clear Slater- and Mott-scenarios and that the orbital degrees of freedom remain quenched even for temperatures above T_N. The d^4-system is already insulating at very high temperatures. Both a crystal field and spin-orbit coupling (SOC) lead to antiferromagnetic order at low temperature, but the finite-T properties differ markedly: Without SOC, the onsite states defining the local moments do not change substantially with $T > T_\mathrm{N}$. In the presence of SOC, in contrast, weight in the onsite singlet favored by SOC increases markedly when T is lowered towards T_N. This is in agreement with X-ray reporting changes to the orbital character at temperatures above T_N.

MA 37.9 Wed 17:15 HSZ 304

Nonlinear spin-wave theory for the Heisenberg-Kitaev model in a magnetic field — •Pedro M. Cônsoli[1,2], Lukas Janssen[2], Matthias Vojta[2], and Eric C. Andrade[1] — [1]Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil — [2]Institut für Theoretische Physik, TU Dresden, Dresden, Germany

The exact solution of Kitaev's honeycomb model and the ensuing realization that it gives rise to chiral Majorana edge modes in a small and properly oriented magnetic field sparked an intense search for a physical mechanism capable of replicating such a system in real materials. This missing link was provided by Khaliullin and Jackeli, who showed that an interplay between crystal field effects and strong spin-orbit coupling originates the Kitaev interaction along with a Heisenberg exchange in a class of Mott insulators. Hence, the Heisenberg-Kitaev Hamiltonian became a minimal model to describe Kitaev materials and was subsequently studied in much detail. Still, several questions related to effects of external perturbations remain unanswered.

Here, we discuss the physics of the Heisenberg-Kitaev model in the presence of a magnetic field applied along two different directions: [100] and [111], for which an intricate classical phase diagram has been reported. In both settings, we employ spin-wave theory for a number of ordered phases to compute magnetization curves and phase boundaries in next-to-leading order in $1/S$, with S being the spin size. In this way, we show that quantum corrections substantially modify the phase diagram. Finally, we compare our spin-wave theory results to exact diagonalization calculations performed on a 24-site cluster.

MA 37.10 Wed 17:30 HSZ 304

How spin-orbital entanglement depends on the spin-orbit coupling in a Mott insulator — •Dorota Gotfryd[1,2], Ekaterina M. Paerschke[3,4], Andrzej M. Oles[2,5], and Krzysztof Wohlfeld[1] — [1]Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [2]Institute of Physics, Jagiellonian University, Lojasiewicza 11, PL-30348 Krakow, Poland — [3]Department of Physics, University of Alabama at Birmingham, Birmingham, Alabama 35294, USA — [4]Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria — [5]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

The concept of spin-orbital entanglement plays a crucial role in understanding various phases and exotic ground states in a broad class of materials, including orbitally ordered materials and spin liquids. We investigate how this entanglement depends on the value of the relativistic spin-orbit coupling. To this end, we numerically diagonalise spin-orbital model with the 'Kugel-Khomskii' exchange supplemented by the on-site spin-orbit coupling. While for small spin-orbit coupling the ground state resembles the vanishing spin-orbit coupling case, for large spin-orbit coupling it can either show negligible spin-orbital entanglement or can evolve to a highly entangled state with completely distinct properties, described by an effective model. The presented range of spin-orbit coupling is relevant not only for 5d but also for 3d or some of the 4d transition metal oxides.