MA 4: Frustrated Magnets - General 1 (joint session TT/MA)

Time: Monday 9:30–13:00 Location: HSZ 304

MA 4.1 Mon 9:30 HSZ 304

Pressure tuning of the ground state of a frustrated Kondo lattice investigated by Muon Spin Relaxation / Rotation spectroscopy — •Mayukh Majumder[1], Ritu Gupta[2], Philipp Gegenwart[1], Oliver Stockert[3], and Veronika Fritsch[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [3]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Formation of novel quantum states driven by magnetic frustration are of strong current interest. For metallic Kondo lattices tuned to a quantum critical point (QCP), strong frustration is predicted to cause a severe breakdown of Fermi liquid behavior and a possible metallic spin liquid state. CePdAl is a prototype frustrated Kondo lattice with incommensurate long-range magnetic order (LRO) at about 2.7 K involving only 2/3-rd of the 4f moments. The LRO can be suppressed by hydrostatic pressure exceeding 1 GPa [1] and an extended non-Fermi liquid ground state has been observed up to a pressure of about 1.7 GPa [2]. We have employed Muon Spin Relaxation / Rotation (μSR) at milli-Kelvin temperatures and pressures up to 1.62 GPa as a local technique to determine the nature of the magnetic moments across the quantum critical point in CePdAl.

[1] H. Kitazawa et al. Phys. B, 28, 199 (1994)
[2] Zhao et al. Nature Phys. 10.1038/s41567-019-0666-6 (2019)

MA 4.2 Mon 9:45 HSZ 304

Microscopic meaning of the Goodenough-Kanamori-Anderson (GKA) rule in frustrated cuprates — •Stefan-Ludwig Drechsler[1], Liviu Hozoi[1], Ravi Yadav[1], Satoshi Nishimoto[1,2], Rolf Schumann[2], Jan M. Tomczak[3], Dijana Miloslavlevic[4], and Helge Rosner[4] — [1]IFW-Dresden, D-01171 Dresden Germany — [2]TU Dresden, Germany — [3]Vienna University of Technology, Vienna, Austria — [4]MPI-cPfS, Dresden, Germany

Within the multiband (pd) Hubbard model we consider the influence of the ferromagnetic (fm) intersite exchange K_{pd} and that of the intra-site Hund's rule exchange J_H on bridging O in between two Cu-sites on the NN exchange J_1 within a spin-model for cuprates with edge-sharing elements. Based on quantum chemistry (QC), DFT, GW, and exact calculations for small clusters and extended systems we determine the main interactions and transfer integrals for several representative cuprates with edge-sharing elements. In most such compounds with Cu-O-Cu bond angles near 90^o the relatively large $-J_1 > 230$ K is dominated by a *nonuniversal* $K_{pd} > 100$ meV, i.e. significantly larger than 50 meV adopted previously /1/. In contrast to common belief, $J_H < 0.8$ eV is moderate and somewhat screened. It plays only a *minor* role in the GKA. Moderate J_H-values are in accord with results for superoxides /2/. Enlarged K_{pd} ~200 meV agree with QC for corner-sharing cuprates /3/ and empirically with $CuGeO_3$ (~ 100 meV) /2/.

[1] Y. Mizuno *et al.*, Phys. Rev. B **57**, 5326 (1998).
[12] M. Matsuda *et al.*, ibid. **100** 104415 (2019) and references therein.
[3] M.S. Hybertsen *et al.*, ibid. **45**, 10032 (1992).

MA 4.3 Mon 10:00 HSZ 304

Magnetic interactions in the new double perovskite Nd_2ZnIrO_6, probed by Resonant Elastic X-ray Scattering (REXS) — •Florian Heinsch[1,2], Morgan Allison[2], Sonia Francoual[3], Jochen Geck[2], Florian Rasch[4], Tobias Ritschel[2], Quirin Stahl[2], Raman Thiyagarajan[1,2], Michael Vogl[4], Eugen Weschke[5], and Sabine Wurmehl[4] — [1]HZDR, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]DESY, Hamburg, Germany — [4]IFW, Dresden, Germany — [5]HZB, Berlin, Germany

The unique interplay of spin-orbit coupling, crystal field splitting and Coulomb repulsion have made double perovskites of the general formula $A_2BB'O_6$ with a 5d transition metal sitting on the B'-site a subject of intense research. Recently a new series Ln_2ZnIrO_6 with Ln = Nd, Sm, Eu and Gd and Ir as 5d-elment could be synthesized [1]. In this series, Nd_2ZnIrO_6 stands out because of its particularly intriguing magnetic properties.

Here we present results of REXS experiments on a Nd_2ZnIrO_6 single crystal, conducted at P09 at PETRA III and UE46 PGM-1 at BESSY. The combined capabilities of both facilities provided us with temperature (down to ~5K) and magnetic magnetic field (up to ~13T) dependent data that elucidate the particularly strong correlation between the two magnetic sublattices of the Nd^{3+} and Ir^{4+} ions. An outlook will be given on how to put the found field dependent anisotropy in a comprehensive picture of the magnetic ground state of Nd_2ZnIrO_6 and how that relates to compounds with different Ln.

[1] M. Vogl et al., arXiv:1910.13552

MA 4.4 Mon 10:15 HSZ 304

Crystal growth and characterization of $ZrFe_4Si_2$ — •Katharina M. Zoch, Isabel Reiser, Alexander Bodach, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany

The crystal structure of $ZrFe_4Si_2$ consists of edge-linked Fe-tetrahedra along the crystallographic *c*-direction. This type of arrangement is prone to show frustration and low dimensional fluctuations. First results indicate that $ZrFe_4Si_2$ displays some sort of weak magnetic order at unusual low temperatures for a Fe-based compound, as well as deviant behavior in specific heat and resistivity measurements [1]. To further investigate these features, we are in need of good quality single crystals. The crystal growth is a challenging subject since the compound is strongly peritectic melting and its melted elements are reactive with common crucible materials under crystal growth conditions. We show first results of the crystal growth from a levitating melt using the Czochralski method. Furthermore, we present the characterization of the obtained samples especially near the suspected magnetic order.

[1] K. Weber: Intermetallic 3d systems close to a magnetic instability: new unusual cases, Dissertation TU Dresden (2017)

MA 4.5 Mon 10:30 HSZ 304

Orientation dependence of the magnetic phase diagram of $Gd_2Ga_5O_{12}$ — •Markus Kleinhans, Christopher Duvinage, and Christian Pfleiderer — Physik-Department, Technische Universität München, D-85748 Garching, Germany

The magnetic properties of $Gd_2Ga_5O_{12}$ (GGG) originate in large, classical spins ($J = S = 7/2$) that interact antiferromagnetically on two interpenetrating hyperkagome lattices. It has long been recognized that this implies, on a classical level, a high degree of frustration with some kind of classical spin liquid at low temperatures. Yet, dipolar interactions are large and may normally be expected to relieve the effects of geometric frustration. Therefore, it has been considered surprising that GGG at zero magnetic field exhibits spin-freezing without evidence for long-range order, where the recent observation of antiferromagnetic correlations on ten-spin rings, suggests a nematic order parameter, or director. We report vibrating coil magnetometry of the orientation dependence of the magnetic phase diagram of GGG down to mK temperatures, where the applied magnetic field stabilizes a complex sequences of cross-overs and phase transitions that reflect the underlying antiferromagnetic interactions.

MA 4.6 Mon 10:45 HSZ 304

Effective chainlike physics in frustrated $S=\frac{1}{2}$ spin-trimer Heisenberg magnets $Na_2Cu_3Ge_4O_{12}$ and $K_2Cu_3Ge_4O_{12}$ — •Oleg Janson[1] and Satoshi Nishimoto[1,2] — [1]Leibniz Institute für Festkörper- und Werkstoffforschung (IFW Dresden) — [2]Technische Universität Dresden (TU Dresden)

The trimerized $S=\frac{1}{2}$ Heisenberg magnet $Na_2Cu_3Ge_4O_{12}$ exhibits an incommensurate magnetic order below $T_N = 2$ K [1], which is nearly two orders of magnitude smaller than the Weiss temperature $\theta_W \simeq 200$ K. Its potassium sibling $K_2Cu_3Ge_4O_{12}$ features similar structural Cu_3O_8 trimers, but their connectivity is different. Here, despite the sizable antiferromagnetic $\theta_W = 49$ K, the magnetic susceptibility $\chi(T)$ reveals no sign of long-range magnetic ordering down to 2.5 K [2]. For both materials, $\chi(T)$ data can not be described within the Heisenberg trimer model. To provide a microscopic insight into the spin models of both materials, we perform microscopic modeling by means of DFT band structure calculations. We find, besides the dominant intertrimer exchange J_1, three (two) further antiferromagnetic exchanges that give rise to a quasi-1D frustrated model in $Na_2Cu_3Ge_4O_{12}$ ($K_2Cu_3Ge_4O_{12}$). The ground states of the spin Hamiltonians are studied using exact diagonalization and DMRG. We also compute the central charge c and the static structure factor $S(q)$, and discuss the possibility to describe the physics of these highly frustrated materials within an effective Heisenberg chain model.

[1] Y. Yasui *et al.*, J. Appl. Phys. **115**, 17E125 (2014).
[2] C. Stoll *et al.*, Inorg. Chem. **57**, 14421 (2018).

MA 4.7 Mon 11:00 HSZ 304

Low-temperature thermal conductivity in the frustrated spin chain mineral Linarite — •Matthias Gillig[1], Xiaochen Hong[1], Gaël Bastien[1], Anja U.B. Wolter[1], Bernd Büchner[1,2], and Christian Hess[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany — [2]Center for Transport and Devices, TU Dresden, Germany

Motivated by recent theoretical results which predict a finite thermal Drude weight in frustrated spin chains, we have studied the thermal conductivity of the mineral Linarite $PbCuSO_4(OH)_2$ at low temperature. This well-studied material forms a monoclinic structure where a sequence of $Cu(OH)_2$ units forms a S=1/2 spin chain. Competing FM nearest-neighbor and AFM next-nearest-neighbor interactions in this low dimensional spin structure create a magnetically frustrated system which orders below $T_N = 2.8$ K in an elliptical spiral ground state. Upon applying magnetic field along the spin chain direction, other magnetically ordered phases can be induced. For fields of 10 T and higher the spin system is fully polarized. Our results reveal that the thermal conductivity κ in zero field is dominated by a phononic contribution. As a function of magnetic field κ shows a peculiar non-monotonic behavior. Whenever the magnetic field value approaches a critical field, κ is highly suppressed. This trend can be explained by strong magnetic fluctuations which are expected near a phase boundary and which reduce thermal conductivity by phonon scattering.

15 min. break.

MA 4.8 Mon 11:30 HSZ 304

Magnetic properties and phase diagram of the triangular-lattice antiferromagnet $KCeS_2$ — •Bastian Rubrecht[1,2], Gael Bastien[1], Anja U.B. Wolter[1], Sven Luther[3], Hannes Kühne[3], Philipp Schlender[4], Ellen Häussler[4], Thomas Doert[4], and Bernd Büchner[1,2] — [1]Institute for Solid State and Materials Research, Leibniz IFW Dresden, Germany — [2]Institute for Solid State and Materials Physics, TU Dresden, Germany — [3]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [4]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany

Triangular-lattice(TL) antiferromagnets are well-known canditates for frustrated magnetism. By introducing different magnetic rare-earth ions, one can change the magnetic interactions to reinforce frustration in these systems. This may lead to the realization of a quantum spin liquid state or to various competing ordered phases, e.g. an oblique version of the 120° state or a collinear up-up-down phase. The delafossite $KCeS_2$ is a new contender realizing anisotropic magnetic interactions. From magnetization measurements of $KCeS_2$-crystals, we observe a strong anisotropy between the basal plane and the c axis. This cannot be explained by g-factor values obtained from single site CASSCF calculations and suggests anisotropic magnetic interactions. Furthermore, our He3 specific heat studies at zero field reveal a phase transition at $T_N = 0.38$ K, which follows a non-monotonous shift as function of an applied in-plane field, resulting in three different magnetic phases in fields up to 9 T. We construct the magnetic phase diagram of $KCeS_2$ and discuss the possible nature of the occurring phases.

MA 4.9 Mon 11:45 HSZ 304

Typical Pure Quantum states and the thermodynamics of highly frustrated quantum magnets — •Andreas Honecker[1] and Alexander Wietek[2] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France — [2]Center for Computational Quantum Physics, Flatiron Institute, New York, USA

Reliable computation of the low-temperature thermodynamic properties of highly frustrated quantum magnets remains a considerable challenge. Here we explore the power of Thermal Pure Quantum (TPQ) states implemented in the framework of a Lanczos method using examples of frustrated two-dimensional $S = 1/2$ spin models. In particular, we present accurate results for the specific heat and magnetic susceptibility 2D $S = 1/2$ Shastry-Sutherland model with up to 40 sites in the parameter regime relevant to $SrCu_2(BO_3)_2$ [1] that had remained inaccessible over the previous two decades.

[1] A. Wietek, P. Corboz, S. Wessel, B. Normand, F. Mila, and A. Honecker, Phys. Rev. Research **1**, 033038 (2019).

MA 4.10 Mon 12:00 HSZ 304

Strain-induced order in highly frustrated magnets — •Mary Madelynn Nayga and Matthias Vojta — Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

One defining feature of highly frustrated magnets is a massively degenerate manifold of classical ground states. Here we study how inhomogeneous strain can lift this degeneracy and induce magnetic order in frustrated magnets. We provide explicit examples of strain-induced ordered states and characterize their observable properties, both static and dynamic.

MA 4.11 Mon 12:15 HSZ 304

Quantum criticality of an extended XY-chain with long-range interactions in a transverse field — •Patrick Adelhardt and Kai Phillip Schmidt — Friedrich-Alexander Universität, Erlangen, Germany

The critical breakdown of a one-dimensional quantum magnet with long-range interactions is studied by investigating an extended XY-model in a transverse field for the ferro- and antiferromagnetic case. While for the the limiting case of the pure long-range XY-model we can extract the elementary one-particle excitation analytically, for the long-range Ising limit as well as in the intermediate regime we use perturbative continuous unitary transformations on white graphs in combination with classical Monte Carlo simulations [1] for the graph embedding on the chain to extract high-order series expansions. This allows us to determine the quantum-critical regime including critical exponents.

[1] S. Fey, S.C. Kapfer, K.P. Schmidt, Phys. Rev. Lett. 122, 017203 (2019)

MA 4.12 Mon 12:30 HSZ 304

Quantum criticality of the transverse-field Ising model with long-range interactions on triangular-lattice cylinders — •Jan Koziol, Sebastian Fey, Sebastian C. Kapfer, and Kai P. Schmidt — Lehrstuhl für Theoretische Physik I, Staudtstraße 7, Universitaet Erlangen-Nuernberg, D-91058 Erlangen, Germany

To gain a better understanding of the interplay between frustrated long-range interactions and zero-temperature quantum fluctuations, we investigate the ground-state phase diagram of the transverse-field Ising model with algebraically decaying long-range Ising interactions on quasi-one-dimensional infinite-cylinder triangular lattices. Technically, we apply various perturbative approaches including low- and high-field series expansions, as well as quantum Monte-Carlo stochastic series expansion simulations. For the classical long-range Ising model, we investigate cylinders with an arbitrary even circumference. We show the occurrence of gapped stripe-ordered phases emerging out of the infinitely degenerate nearest-neighbor Ising ground-state space on the two-dimensional triangular lattice. For the full long-range transverse-field Ising model, we concentrate on cylinders with circumference four and six. The ground-state phase diagram consists of several quantum phases in both cases including an x-polarized phase, stripe-ordered phases, and clock-ordered phases which emerge from an order-by-disorder scenario already present in the nearest-neighbor model. In addition, the generic presence of a potential intermediate gapless phase with algebraic correlations and associated Kosterlitz-Thouless transitions is discussed for both cylinders.

MA 4.13 Mon 12:45 HSZ 304

Dynamic Structure Factor of Disordered Coupled-Dimer Heisenberg models — •Max Hörmann and Kai Phillip Schmidt — Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstraße 7, D-91058 Erlangen

We investigate the impact of quenched disorder on the zero-temperature dynamic structure factor of coupled-dimer Heisenberg models on two-dimensional bilayers on the square, triangular and Kagome lattice. Using perturbative continuous unitary transformations, the effects on quasiparticles are investigated [1]. The disorder leads to intriguing quantum structures in dynamical correlation functions well observable in spectroscopic experiments.

[1] M. Hörmann, P. Wunderlich, K. P. Schmidt, Phys. Rev. Lett. 121, 167201 (2018)