TT 72: Correlated Electrons: Frustrated Magnets - General 2

Time: Thursday 15:00–18:30 Location: HSZ 204

TT 72.1 Thu 15:00 HSZ 204

The role of nonmagnetic d0 vs d10 B-type cations on the magnetic exchange interactions in osmium double perovskites — •Hai Feng[1], Kazunari Yamaura[2], Martin Jansen[3], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids — [2]National Institute for Materials Science — [3]Max Planck Institute for Solid State Research

Double perovskite oxides, A2BB'O6, containing 4d/5d elements have attracted considerable attention due to their remarkable electronic and magnetic properties, such as room-temperature magnetoresistance and high-temperature ferrimagnetism. In this talk, we will present our studies on the magnetic properties of osmium double perovskite oxides Ba2BOsO6 (B = Sc, Y, In). Ba2BOsO6 (B = Sc, Y, In) adopt the cubic double perovskite structures (space group, Fm-3m) with ordered B and Os arrangements and show antiferromagnetic transitions at 93 K, 69 K, and 28 K, respectively. The Weiss-temperatures are -590 K for Ba2ScOsO6, -571 K for Ba2YOsO6, and -155 K for Ba2InOsO6. Sc3+ and Y3+ have the open-shell d0 electronic configuration, while In3+ has the closed-shell d10. This indicates that a d0 B-type cation induces stronger overall magnetic exchange interactions in comparison to a d10. Comparison of Ba2BOsO6 (B = Sc, Y, In) to their Sr and Ca analogues shows that the structural distortions weaken the overall magnetic exchange interactions.

TT 72.2 Thu 15:15 HSZ 204

Magnetic properties of A_2TaCl_6 with $5d^1$ electons on FCC lattice — •Hajime Ishikawa[1], Tomohiro Takayama[2], Robert Dinnebier[2], and Hidenori Takagi[2] — [1]University of Stuttgart, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

$5d$ transition metal compounds are expected to show exotic magnetism as a result of the interplay between electronic correlation and strong spin-orbit coupling. In the case of $5d^1$ electronic configuration, the electron is considered to occupy the $J_{eff} = 3/2$ states, where effective orbital angular momentum $L_{eff} = 1$ and spin angular momentum $S = 1/2$ cancel with each other. In recent theoretical studies, rich ground states are predicted in the system where localized electrons in $J_{eff} = 3/2$ states are arranged on the face centered cubic (FCC) lattice. Experimentally, several double perovskite oxides with FCC lattice have been studied as a model compound, however, their spin and orbital states are still unclear and under debate. The FCC lattice made of transition metal ions are also found in a series of halides with the chemical formula A_2MX_6. In this study, we studied physical properties of A_2TaCl_6 with $5d^1$ electronic configuration and their related materials by means of magnetization and heat capacity measurements and low-temperature X-ray diffraction experiments. Based on the results, we discuss the spin-orbital state of Ta^{4+} ion and difference between oxides and halides.

TT 72.3 Thu 15:30 HSZ 204

ESR Spectroscopy on the Coupled Spin Tetrahedral System $Cu_2Te_2O_5Cl_2$ — •Julian Zeisner[1,2], Vladislav Kataev[1], Mirta Herak[3], Dijana Zilic[4], Helmuth Berger[5], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, Germany — [3]Institute of Physics, Zagreb, Croatia — [4]Rudjer Boskovic Institute, Zagreb, Croatia — [5]Institut de Physique de la Matière Complexe, EPFL, Lausanne, Switzerland

Systems with reduced dimensionality and magnetic frustration gained considerable attention in modern solid state research as both phenomena individually lead to an enhancement of the impact of fluctuations on magnetic properties and low-energy excitations. The coupled spin tetrahedral compound $Cu_2Te_2O_5Cl_2$ belongs to a class of materials which allow to study the interplay of both effects. In our work we performed a high-field high-frequency ESR study in order to investigate the magnetic anisotropies present in this system as well as the spin dynamics of the compound. Measurements were conducted over a wide frequency and temperature range revealing a small g-factor anisotropy at room temperature which is consistent with torque magnetometry results. Furthermore, the temperature dependence of the linewidth indicates the onset of slowing down of spin fluctuations far above the ordering temperature.

TT 72.4 Thu 15:45 HSZ 204

J_1-J_2 Heisenberg model on a triangular-lattice bilayer — •Darshan G. Joshi[1] and Matthias Vojta[2] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

We consider a triangular-lattice bilayer Heisenberg model for spins 1/2 with antiferromagnetic nearest-neighbor and next-nearest-neighbor interactions. We determine the phase diagram and the dispersion of elementary excitations using variants of bond-operator theory. Large inter-layer coupling yields a dimer quantum paramagnet, while magnetic order is possible for weak inter-layer coupling. Frustration can induce flat portions of triplon bands in the dimer phase, opening the window to find exotic states in the vicinity to the transition point to ordered phases. For weak inter-layer coupling we reproduce the possible spin-liquid state known from the single-layer J_1-J_2 model which occurs when 120° order is destroyed by increasing J_2. Remarkably, this state is destabilized in favor of magnetic order with increasing inter-layer coupling before amplitude fluctuations destroy magnetic order at large inter-layer coupling.

TT 72.5 Thu 16:00 HSZ 204

Quantum domain walls induce incommensurate supersolid phase on the anisotropic triangular lattice — •Xue-Feng Zhang[1,2], Shijie Hu[2], Axel Pelster[2], and Sebastian Eggert[2] — [1]Max-Planck- Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

We investigate the extended hard-core Bose-Hubbard model on the triangular lattice as a function of spatial anisotropy with respect to both hopping and nearest-neighbor interaction strength [1]. At half filling the system can be tuned from decoupled one-dimensional chains to a two-dimensional solid phase with alternating density order by adjusting the anisotropic coupling. At intermediate anisotropy, however, frustration effects dominate and an incommensurate supersolid phase emerges, which is characterized by incommensurate density order as well as an anisotropic superfluid density. We demonstrate that this intermediate phase results from the proliferation of topological defects in the form of quantum bosonic domain walls. Accordingly, the structure factor has peaks at wave vectors, which are linearly related to the number of domain walls in a finite system in agreement with extensive quantum Monte Carlo simulations. We discuss possible connections with the supersolid behavior in the high-temperature superconducting striped phase.

[1] Phys. Rev. Lett. 117, 193201 (2016)

TT 72.6 Thu 16:15 HSZ 204

Character of the Néel Transition of Triangular Antiferromagnet $PdCrO_2$ — •Jack Bartlett[1,2], Dan Sun[1], Jhuma Sannigrahi[1], Pallavi Kushwaha[1], Andrew Mackenzie[1,2], and Clifford Hicks[1] — [1]Max-Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, Dresden, 01187, Germany — [2]Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS, United Kingdom

The transition from paramagnetism to antiferromagnetism is usually second-order, but can be driven first-order through magnetoelastic coupling or fluctuation effects. In this talk, we present data on the antiferromagnetic transition of $PdCrO_2$. This is a layered, triangular compound consisting of alternating sheets of highly conductive Pd and insulating, magnetic CrO_2. The Cr spins are Heisenberg-like, and below $T_N \sim 38$ K order into the the 120° Néel phase. Resistivity data on uniaxially-stressed $PdCrO_2$ suggest that at zero stress the transition is weakly first-order, however on close inspection the transition appears to be a crossover. We discuss further using resistivity, thermal expansion, and susceptibility data.

TT 72.7 Thu 16:30 HSZ 204

The response of a triangular antiferromagnet to anisotropic lattice distortion — •Dan Sun[1], Jack Bartlett[1,2], Jhuma Sannigrahi[1], Pallavi Kushwaha[1], Andrew Mackenzie[1,2], and Clifford Hicks[1,2] — [1]Max-Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, Dresden, 01187, Germany — [2]Scottish Uni-

versities Physics Alliance (SUPA), School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS, United Kingdom

The ground state of Heisenberg spins interacting antiferromagnetically on a triangular lattice is 120° antiferromagnetic order. We probe the effects of anisotropic lattice distortion on this phase using the material $PdCrO_2$, which has highly-conducting Pd sheets that alternate with Mott-insulating CrO_2 layers. The Cr spins order into a 120° phase at T_N = 39 K. The conductivity of the Pd sheets can be measured to probe magnetic scattering across the transition. In the unstrained lattice, the resistivity has a sharp first-order-like step at T_N. It persists with almost no change up to a compression of $\sim$ 0.2%, then broadens dramatically. This feature suggests a rigidity of the 120° phase at $T \sim T_N$ against small perturbations, which we discuss in terms of magnetoelastic coupling and fluctuation effects.

15 min. break.

TT 72.8 Thu 17:00 HSZ 204

Non-Abelian Symmetries in Tensor Network Algorithms — •Philipp Schmoll[1,2] and Román Orús[1] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany

In recent years Tensor Networks (TNs) have emerged as a natural language to describe quantum states of matter by capturing the amount and local structure of entanglement in the system. They provide an efficient framework to study quantum many-body properties with many remarkable applications such as the Density Matrix Renormalization Group (DMRG) for 1d systems proposed by S. White. The Projected Entangled Pair State (PEPS) ansatz has proven to be a versatile tool for 2d systems with topological order, both chiral and non-chiral. However, at the current stage simulations in 2d are strongly limited due to the complexity of the systems. In this respect, a big step needs to be taken to have a versatile implementation of non-abelian symmetries (such as SU(2) or SU(3)) in 2d PEPS algorithms, which will allow to advance significantly in the study of many relevant systems (e.g., frustrated antiferromagnets, chiral topological spin liquids, ...). In this talk I will report on recent advances in this direction at our group in Mainz.

TT 72.9 Thu 17:15 HSZ 204

The spin-1/2 Kagome XXZ model in a field: competition between lattice nematic and solid orders — •Augustine Kshetrimayum[1], Thibaut Picot[2], Román Orús[1], and Didier Poilblanc[2] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Laboratoire de Physique Théorique, IRSAMC, CNRS and Université de Toulouse, UPS, F-31062 Toulouse, France

We study numerically the spin-1/2 XXZ model in a field on an infinite Kagome lattice. We use different algorithms based on infinite Projected Entangled Pair States (iPEPS) for this, namely: (i)an approach with simplex tensors and 9-site unit cell, and (ii) an approach based on coarse-graining three spins in the Kagome lattice and mapping it to a square-lattice model with local and nearest-neighbor interactions, with usual PEPS tensors, 6- and 12-site unit cells. We observe the emergence of several magnetization plateaus as a function of the field for different values of the anisotropy. We focus on the 1/3 plateaus using both the techniques and study the nature of its ground state as we tune the anisotropy from the Ising regime to the XY regime through the Heisenberg point and find a strong competition between lattice nematic and solid orders.

TT 72.10 Thu 17:30 HSZ 204

Magnetic properties of Li_2FeSiO_4 single crystals — •Fabian Billert, Johannes Werner, Christoph Neef, Changhyun Koo, and Rüdiger Klingeler — Kirchhoff Institute of Physics, Heidelberg University, Heidelberg

Li_2FeSiO_4 single crystals of the high-temperature *Pmnb*-phase were grown by means of the travelling-solvent floating-zone technique. The single-crystal structure refinement reveals corner-sharing FeO_4 and SiO_4 tetrahedra in the *ac*-layers. Static magnetisation studies reveal long-range antiferromagnetic order below T_N = 17 K. The maximum of the magnetic suceptibility appears at around 25 K indicating significant antiferromagnetic correlations well above T_N. This is corroborated by means of high-frequency electron spin resonance (HF-ESR) measurements which show temperature dependent resonances, i.e. the evolution of local magnetic fields, up to 100 K. Below T_N, antiferromagnetic resonance modes are detected and significant zero-field splitting is observed.

TT 72.11 Thu 17:45 HSZ 204

Strong coupling on structure and magnetism in $SrCo_2P_2$ — •Inga Kraft[1,2], Kathrin Götze[3,2], Johannes Klotz[3], Vivien Lorenz[4], Christoph Bergmann[1], Yurii Prots[1], Jan Bruin[5], Alix McCollam[5], Ilya Sheikin[6], Jochen Wosnitza[2], Christoph Geibel[1], and Helge Rosner[1] — [1]MPI CPfS, Dresden — [2]Technical University of Dresden — [3]HLD-EMFL, Dresden — [4]Institut für Festkörper- und Werkstoffforschung (IFW), Dresden — [5]HFML-EMFL, Nijmegen, The Netherlands — [6]CNRS Grenoble, France

Though the iron pnictide 122 systems show a comparatively simple structure, they attracted large interest owing to their rich physics. $SrCo_2P_2$ is closely related to the iron-pnictide superconductors, but does not show superconductivity or magnetic order down to 300 mK. In contrast, previous DFT band structure calculations found a large DOS at E_F and predicted a magnetic (or other) instability. Based on new low temperature XRD structural data, we calculate the respective electronic structure and compare it to the angle-dependent dHvA measurements. Our results yield a strongly reduced DOS(E_F) and explain the observed strong magnetic fluctuations and absence of magnetic order.

TT 72.12 Thu 18:00 HSZ 204

Spin liquid and quantum phase transition without symmetry breaking in a frustrated three-dimensional Ising model — •Kai Phillip Schmidt[1], Julia Roechner[2], and Leon Balents[3] — [1]FAU Erlangen-Nürnberg, Erlangen, Germany — [2]TU Dortmund, Dortmund, Germany — [3]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, USA

We show that the highly frustrated transverse-field Ising model on the three-dimensional pyrochlore lattice realizes a first-order phase transition without symmetry breaking between the low-field Coulomb quantum spin liquid and the high-field polarized phase. The quantum phase transition is located quantitively by comparing low- and high-field series expansions. Furthermore, the intriguing properties of the elementary excitations in the polarized phase are investigated. We argue that this model can be achieved experimentally by applying mechanical strain to a classical spin ice material comprised of non-Kramers spins such as $Ho_2Ti_2O_7$. Taken together with our results, this provides a new experimental platform to study quantum spin liquid physics.

TT 72.13 Thu 18:15 HSZ 204

Magnetism of correlated covalent insulator $SrRu_2O_6$ — Atsushi Hariki and •Jan Kuneš — TU Wien, Austria

We present a density functional + dynamical mean-field theory (LDA+DMFT) study of $SrRu_2O_6$. Considering the interaction strength this d^3 material is on the correlated-metal side of the Mott transition. Special hopping pattern, however, gives rise to pronounced molecular orbital features and results in opening of a hybridization gap. The physics is governed by a competition between localization and covalency in a half-filled Hund's material.