TT 12: Correlated Electrons: Frustrated Magnets - General 1

Time: Monday 15:00–18:15 Location: HSZ 03

TT 12.1 Mon 15:00 HSZ 03

Excitations of the Shastry-Sutherland model in the plaquette phase — •Carolin Boos[1], Frédéric Mila[2], and Kai Schmidt[1] — [1]FAU Erlangen-Nürnberg, Deutschland — [2]EPF Lausanne, Schweiz

The quantum magnet $SrCu_2(BO_3)_2$ is well described by the two-dimensional Shastry-Sutherland model, that is a frustrated spin-1/2 system on a square lattice with some next-nearest-neighbor interactions. Under pressure a quantum phase transition is observed in $SrCu_2(BO_3)_2$, which is suggested to correspond to the plaquette phase of the Shastry-Sutherland model. In this work we study the excitation spectrum of the plaquette phase to clarify the presence of this phase in $SrCu_2(BO_3)_2$.
To this end we consider a high-order linked-cluster expansion using perturbative continous transformations about the isolated plaquette limit. We calculate the dispersion and compare it with inelastic neutron scattering results of $SrCu_2(BO_3)_2$ under a pressure of 21.5 kbar from [1].

[1] M.E. Zayed *et al.*, ArXiv:1603.02039v1, 2016.

TT 12.2 Mon 15:15 HSZ 03

Anisotropic kagome lattice as the origin of canted antiferromagnetism in barlowite — •Alexander A. Tsirlin[1], Ronald Zinke[2], Ioannis Rousochatzakis[3], Helge Rosner[4], and Johannes Richter[2] — [1]EP VI, EKM, University of Augsburg, Germany — [2]Institute of Theoretical Physics, University of Magdeburg, Germany — [3]School of Physics, University of Minnesota, Minneapolis, US — [4]MPI for Chemical Physics of Solids, Dresden, Germany

Barlowite is a recent addition to the family of spin-$\frac{1}{2}$ kagome minerals that, despite its reported three-fold symmetry of the crystal structure, reveals long-range magnetic order below 15 K with a weak remnant magnetization. Using density-functional band-structure calculations along with the effective theory and coupled-cluster method for spin Hamiltonians, we propose that the disordered arrangement of the interlayer Cu site gives rise to a tangible deformation of the kagome layers. Their local configurations can be represented by a combination of weakly coupled linear trimers and spatially anisotropic kagome lattice. While the former give rise to simple antiferromagnetic order, the latter supports canted antiferromagnetic order driven by quantum fluctuations and reinforced by Dzyaloshinsky-Moriya anisotropy. This mechanism stabilizes canted antiferromagnetic order with a relatively low net moment lying in the kagome plane, which is only possible when geometrical distortion of the kagome lattice is taken into account.

TT 12.3 Mon 15:30 HSZ 03

Magnetic resonance as a local probe for $S = \frac{1}{2}$ Kagomé magnetism in Barlowite $Cu_4(OH)_6FBr$ — •Ranjith Kumar Kizhake Malayil[1], Christian Klein[2], Cornelius Krellner[2], and Michael Baenitz[1] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Institute of Physics, Goethe-University Frankfurt, 60438 Frankfurt am Main, Germany

$S = \frac{1}{2}$-quantum magnets with Kagomé 2D layer building blocks could serve as model systems for 2D magnetic frustration and may host the quantum spin liquid state (QSL). So far Herbertsmithite (HS) $ZnCu_3(OH)_6Cl_2$ is the leading candidate for this research, but here structural disorder has some influence on the QSL state. Barlowite, $Cu_4(OH)_6FBr$ is a relative to HS and is predicted to host an undistorted Kagomé lattice [1].

Here, we present ^{1}H, ^{19}F, and ^{79,81}Br NMR measurements together with a Br-NQR study on polycrystalline samples to probe the magnetism, the magneto elastic coupling and the local disorder. From spin-lattice relaxation results strong evidence for magnetic order at 15 K is given. Furthermore, a large field dependence of the hyperfine fields is observed. This is discussed to originate from a weak out of plane magnetic exchange interaction.

[1] Han et al., Phys. Rev. Lett. **113**, 227203 (2014).

TT 12.4 Mon 15:45 HSZ 03

Electronic Excitations and Lattice Vibrations on the Kagome Lattice: Herbertsmithite and Related Compounds — •Andrej Pustogow[1], Mathias Bories[1], Ievgen Voloshenko[1], Pascal Puphal[2], Cornelius Krellner[2], Ying Li[2], Roser Valenti[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Physikalisches Institut, Universität Frankfurt

We present a broadband optical and theoretical study of the electrodynamic response of the quantum spin liquid candidate Herbertsmithite and related Kagome lattice compounds. At low frequencies the spectrum of these frustrated Mott insulators is dominated by phonons. We assign the lattice vibrations within and perpendicular to the Kagome layer on the basis of theoretical calculations. In the visible and ultraviolet ranges we identify interband transitions and relate them to recent band structure calculations. Finally, we tackle the open question about the theoretically predicted contribution of spinon excitations to the low-frequency optical conductivity.

TT 12.5 Mon 16:00 HSZ 03

New kagome systems $YCu_3(OH)_6Cl_3$ and $Ga_xCu_{4-x}(OH)_6Cl_2$ — •Pascal Puphal[1], Michael Bolte[1], Denis Sheptyakov[2], Andrej Pustogow[3], Martin Dressel[3], Michael Baenitz[4], and Cornelius Krellner[1] — [1]Goethe-University Frankfurt am Main — [2]Laboratory for Neutron Scattering and Imaging, PSI, Villigen — [3]1. PI, Stuttgart University — [4]MPI-CPfS, Dresden

Herbertsmithite $ZnCu_3(OH)_6Cl_2$ is a highly frustrated kagomé system, which has an antiferromagnetic superexchange interaction of J = 17 meV, but no long-range order has been observed down to T = 50 mK. We have successfully prepared $Ga_xCu_{4-x}(OH)_6Cl_2$, with a three valent ion instead of Zn^{2+}, which should lead to a Dirac metal as proposed by I. I. Mazin et. al. [1]. We synthesized powder samples of this compound with different substitution amounts of $x < 1$. Similar to Zn the increasing Ga amount slowly suppresses the ordering at 6.5 K, but the compound stays insulating which is also reflected in its green colour. We show magnetometry, specific heat as well as optical and local probing data like NMR. The second part of the contribution is about $YCu_3(OH)_6Cl_3$ which shows a new kapellasite like structure. Using hydrothermal growth we synthesized single crystals of up to 2 x 2 x 0.5 mm. The structure is a slightly distorted kagome layer with two copper positions giving a new two-dimensional frustrated arrangement. The susceptibility as well as specific heat show a weak antiferromagnetic ordering at 2.2 K while the system has a Weiss temperature of -104 K resulting in a frustration coefficient of 50.

[1] I. I. Mazin et al., Nature Communications 5, 4261 (2014)

TT 12.6 Mon 16:15 HSZ 03

Spin Frustration in an Organic Radical Ion Salt Based on a Kagome-Coupled Chain Structure — •Lars Postulka[1], Stephen M. Winter[1], Bernd Wolf[1], Adam G. Mihailov[2], Aaron Mailman[2], Adbeljalil Assoud[2], Craig M. Robertson[3], Richard T. Oakley[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe Universität, SFB/TR49, Frankfurt, DE — [2]Dep. of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada — [3]Dep. of Chemistry, University of Liverpool, Liverpool L69 7ZD, United Kingdom

Frustrated quantum spin systems have attracted enormous interest in experimental and theoretical studies as these systems are expected to host spin liquid states. A model system for such frustrated quantum magnets is the kagome lattice with S=1/2 moments at the lattice vertices. Here we present a purely organic variant built out of quinoidal bisdithiazole $[BT]^+$ radicals and $[GaBr_4]^-$.The packing pattern of the radical cations provides a rare example of an organic kagome basket structure. Magnetic measurements over a wide temperature range 30 mK $< T <$ 300 K suggest strongly frustrated AFM interactions of the scale of $J/k_B \approx 30$ K, but reveal no anomalies that would be associated with magnetic order. The high-temperature part of the susceptibility can be described in a coupled-chain model. By combining results from high-temperature series expansion and density functional theory we could resolve that these chains are coupled in a distorted kagome lattice[1].

[1] L. Postulka et al., J. Am. Chem. Soc. 138, 10738 (2016)

15 min. break.

TT 12.7 Mon 16:45 HSZ 03

Anisotropy governed competition of magnetic phases in the honeycomb quantum magnet $Na_3Ni_2SbO_6$ — •Johannes Werner[1], Waldemar Hergett[1], Mario Gertig[1], Jaena Park[1],

Changhyun Koo[1], and Rüdiger Klingeler[1,2] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Centre for Advanced Materials, Heidelberg University, Heidelberg, Germany

Thermodynamic properties as well as low-energy magnon excitations of the layered $S = 1$ honeycomb-lattice system $Na_3Ni_2SbO_6$ have been studied by high-resolution dilatometry, high-field magnetometry, and antiferromagnetic resonance (AFMR) studies in magnetic fields up to 18 T. At $T_N = 16.5$ K, there is a tricritical point separating two antiferromagnetic phases AF1 and AF2 from the paramagnetic regime. In the AF1 phase below $B_{C1} \approx 9.5$ T (at 4.2 K), the AFMR modes suggest a two-sublattice spin configuration which is consistent with stripe-like order. Observed zero field splitting $\Delta_{ZFS} = 360$ GHz of the AFMR modes indicates an uniaxial anisotropy field $B_A = 1.7$ T. We conclude the crucial role of the axial anisotropy favoring the AF1 spin structure over the AF2 one. While magnetostriction data disprove a simple spin-flop scenario at B_{C1}, the nature of a second transition at $B_{C2} \approx 13$ T remains unclear. Both the sign of the magnetostriction dL/dB and Grüneisen scaling suggest that short-range antiferromagnetic correlations present at least up to $\sim 5 \cdot T_N$ are of AF2-type, i.e. the intermediate field phase.

TT 12.8 Mon 17:00 HSZ 03

Quantum anomalous Hall state in ferromagnetic $SrRuO_3$ (111) bilayers — Liang Si[1], •Oleg Janson[1], Gang Li[1], Zhicheng Zhong[2], Zhaoliang Liao[3], Gertjan Koster[3], and Karsten Held[1] — [1]Institut für Festkörperphysik, TU Wien, Vienna, Austria — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

We study electronic, magnetic and topological properties of the honeycomb lattice formed by $SrRuO_3$ (111) bilayers by means of density functional theory, dynamical mean field theory (DMFT) and model simulations. DMFT yields a half-metallic ferromagnetic state below 500 K with an ordered magnetic moment of $2\,\mu_B$. In the minority channel, the spin-orbit coupling opens a gap at the linear band crossing corresponding to 4/3 filling of the $4d$ t_{2g} shell. Using model calculations, we demonstrate that the respective state is a quantum anomalous Hall state and discuss possible routes towards an experimental realization of this topological states.

OJ acknowledges the support by the Lise Meitner Programme of Austrian Science Fund (FWF), project M2050.

Invited Talk TT 12.9 Mon 17:15 HSZ 03

U(1) Quantum Spin Liquid Ground State in the Triangular Antiferromagnet $YbMgGaO_4$ — •Yuesheng Li — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg

Quantum spin liquids are novel phases of matter, where spins are entangled up to long-distances and times without symmetry breaking even at 0 K due to the strong quantum fluctuations. And the candidate materials were actively sought after. However, most of the existing candidates suffer from magnetic defect, lattice distortion, antisymmetric exchange (Dzyaloshinskii-Moriya interactions) and (or) interlayer magnetic coupling. Recently, a new structurally perfect triangular antiferromagnet $YbMgGaO_4$ was reported by our group [1,2]. The aforementioned structural shortcomings are avoided [1]. (1) No spin symmetry breaking is detected down to 0.048 K [1,3], and the spin entropy is precisely measured to be almost zero at 0.06 K [1]. (2) The measured magnetic heat capacity behaves as $C_m \sim T^{2/3}$ down to 0.06 K under 0 T [1]. (3) The muon spin relaxation rates exhibit temperature-independent plateaus below 0.4 K [3]. (1)-(3) suggest $YbMgGaO_4$ may be the first experimental realization of the U(1) quantum spin liquid ground state.

[1] Yuesheng Li et al., Sci. Rep. 5, 16419 (2015)
[2] Yuesheng Li et al., Phys. Rev. Lett. 115, 167203 (2015)
[3] Yuesheng Li et al., Phys. Rev. Lett. 117, 097201 (2016)

TT 12.10 Mon 17:45 HSZ 03

Tuning the Effective Correlations in a Mott Insulator and Quantum Spin Lquid Compound — Miriam Sanz Alonso[1], Andrej Pustogow[1], Yohei Saito[2], Atsushi Kawamoto[2], and •Martin Dressel[1] — [1]1. Phys. Inst. Univ. Stuttgart, Germany — [2]Div. of Phys. Hokkaido Univ., Sapporo, Japan

The fictitious state of a quantum spin liquid was first realized in the dimerized Mott system κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ about a decade ago. Here we tune the effective correlations U/W by a gradual increase of the bandwidth W in the substitutional series κ-(BEDT-TTF$_{1-x}$BEDT-STF$_x$)$_2$Cu$_2$(CN)$_3$ with $0 \leq x \leq 1$, where on one side of the molecule sulfur has been replaced by the larger selenium atoms. Comprehensive optical and transport investigations down to low temperatures evidence a metal-insulator transition as x exceeds 20% with no indications that disorder plays a crucial role. We analyze the dynamics of the correlated charge carriers and the shift of spectral weight; the results allow us to generate a unified phase diagram of this Mott system, that remains a spin liquid as it does not exhibit magnetic order down to lowest temperatures.

TT 12.11 Mon 18:00 HSZ 03

Quantum Monte-Carlo study of hardcore bosons on a kagome lattice — •Xue-Feng Zhang[1], Yin-Chen He[2], Sebastian Eggert[3], Roderich Moessner[1], and Frank Pollmann[1] — [1]Max-Planck- Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA — [3]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

We study an extended Hubbard model of hardcore bosons on the kagome lattice. In the limit of strong nearest-neighbor interactions at one-third filling, the interplay between frustration and quantum fluctuation is know to form a valence bond solid. When decreasing the interaction strength, the system has a transition to a superfluid phase. The precise nature of this phase transition is still under debate. Two possibilities are that it could be a weakly first order or an unconventional continuous phase transition. We revisit this problem using large scale quantum Monte Carlo simulation with parallel tempering. We find a first order phase transition away from the tip of the one third filling lobe, while it appears to be continuous at exactly one third filling. A careful finite size scaling analysis reveals an unconventional scaling behavior hinting at deconfined quantum criticality.