TT 18: Frustrated Magnets

Time: Thursday 10:00–12:45 Location: H7

TT 18.1 Thu 10:00 H7

Magnon Crystallization in the Kagome Lattice Antiferromagnet — •Jürgen Schnack[1], Jörg Schulenburg[2], Andreas Honecker[3], and Johannes Richter[4] — [1]Fakultät für Physik, Universität Bielefeld, Postfach 100131, D-33501 Bielefeld, Germany — [2]Universitätsrechenzentrum, Universität Magdeburg, D-39016 Magdeburg, Germany — [3]Laboratoire de Physique Theorique et Modelisation, CNRS UMR 8089, CY Cergy Paris Universite, F-95302 Cergy-Pontoise Cedex, France — [4]Institut für Physik, Universität Magdeburg, P.O. Box 4120, D-39016 Magdeburg, Germany & Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany

We present numerical evidence for the crystallization of magnons below the saturation field at nonzero temperatures for the highly frustrated spin-half kagome Heisenberg antiferromagnet [Phys. Rev. Lett. 125, 117207 (2020)]. This phenomenon can be traced back to the existence of independent localized magnons or, equivalently, flatband multimagnon states. We present a loop-gas description of these localized magnons and a phase diagram of this transition, thus providing information for which magnetic fields and temperatures magnon crystallization can be observed experimentally. The emergence of a finite-temperature continuous transition to a magnon crystal is expected to be generic for spin models in dimension D > 1 where flatband multimagnon ground states break translational symmetry.

TT 18.2 Thu 10:15 H7

Coexistence of static and dynamic spins in the new Kitaev iridate β-$ZnIrO_3$ — •Aleksandr Zubtsovskii and Alexander A. Tsirlin — EP VI, EKM, University of Augsburg, Germany

The three-dimensional Kitaev iridate β-Li_2IrO_3 shows complex magnetic behavior caused by the exchange anisotropy and frustration, and serves as a suitable ground to seek new materials with spin-liquid physics. Here, we report the detailed study of magnetic properties in the new Kitaev compound, β-$ZnIrO_3$, prepared by the low-temperature topotactic ion exchange reaction. The crystal structure characterized by x-ray and neutron diffraction as well as high-resolution electron microscopy exhibits symmetry lowering with respect to the parent β-Li_2IrO_3, but no structural disorder. Magnetic behavior is studied using magnetization and heat capacity measurements as well as μSR. The results indicate spin freezing below $T_f \sim 5$ K and a broad fluctuating regime that extends up to 40 K.

TT 18.3 Thu 10:30 H7

Spin-orbit coupled Mott insulator, Sr_2IrO_4: spin and charge orders — •Mehdi Biderang[1], Alireza Akbari[2], and Jesko Sirker[1] — [1]Department of Physics and Astronomy, University of Manitoba, Winnipeg, Manitoba, Canada R3T 2N2 — [2]Max Planck Institute for the Chemical Physics of Solids, D-01187 Dresden, Germany

An antisymmetric spin-orbit coupling of a two-dimensional single-band Hubbard Hamiltonian is investigated. We propose that this is the most basic paradigm for understanding the electrical characteristics of locally noncentrosymmetric transition metal (TM) oxides like Sr_2IrO_4. Based on exact diagonalizations of small clusters and the random-phase approximation, we study the correlation effects on charge and magnetic order as a function of doping and of the TM-oxygen-TM bond angle. We see dominating commensurate in-plane antiferromagnetic fluctuations for low doping and small angles, whereas ferromagnetic fluctuations dominate for larger angles. Moderately strong nearest-neighbor Hubbard interactions can also stabilize a charge density wave order. We find good qualitative agreement between the dispersion of magnetic excitations in the hole-doped scenario and resonant inelastic x-ray scattering measurements.

TT 18.4 Thu 10:45 H7

Two-triplon excitations in frustrated bilayer systems — •Erik Wagner and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Braunschweig, Germany

We study the magnetism of frustrated bilayer spin models. Starting from the limit of decoupled dimers we use the perturbative continuous unitary transformation (pCUT), based on the flow equation method, to perform series expansion in order to analyze the spectrum, up to the two-triplon excitations. First we apply this method to the Kitaev-Heisenberg bilayer, consisting of two honeycomb Kitaev spin-models with anisotropic intralayer Ising-exchange $J_{x,y,z}$, coupled by additional interlayer Heisenberg exchange J. We evaluate the groundstate energy and the one particle dispersion up to 9th order in $J_{x,y,z}$ as well as the two-particle interactions and spectrum up to 6th order [1]. We detail the presence of (anti-)bound two-particle states and analyze their wavefunctions. Additionally we discuss the impact of two-particle interactions on the magnetic Raman response of the Kitaev-Heisenberg bilayer. Extensions of our approach to other frustrated bilayers will be considered, focusing on the $SU(2)$ invariant J-J_1-J_2-Heisenberg square-lattice bilayer and including calculations up to 7th and 4th order in $J_{1,2}$ for one- and two-particle matrix elements.

[1] E. Wagner, W. Brenig, arXiv:2103.13402

15 min. break.

TT 18.5 Thu 11:15 H7

Anisotropy of the magnetoelastic coupling investigated in the Kitaev material $RuCl_3$ — •Vilmos Kocsis[1], David A. S. Kaib[2], Kira Riedl[2], Sebastian Gass[1], Paula Lampen-Kelley[3,4], David G. Mandrus[3,4], Stephen E. Nagler[4], Nicolas P. Rodriguez[1], Kornelius Nielsch[1], Roser Valenti[2], Bernd Büchner[1], and Anja U. B. Wolter[1] — [1]IFW-Dresden, Dresden, Germany — [2]Goethe-Universität Frankfurt, Frankfurt, Germany — [3]University of Tennessee, Knoxville, USA — [4]Oak Ridge National Laboratory, Oak Ridge, USA

The Kitaev material α-$RuCl_3$ is among the most promising candidates to host a quantum spin-liquid state. Recent investigations have revealed the importance of the magnetoelastic coupling and the magnetic anisotropy in α-$RuCl_3$. In this combined theoretical and experimental research we investigate the anisotropic magnetic and magnetoelastic properties for magnetic fields applied along the main crystallographic axes as well as for fields canted out of the honeycomb plane. We found that the magnetostriction anisotropy is unusually large compared to the anisotropy of the magnetization, which is related to the strong magnetoelastic $\widetilde{\Gamma}'$-type coupling in our *ab-initio* derived model. We observed large, non-symmetric anisotropy in the magnetic and magnetoelastic properties for magnetic fields canted out of the honeycomb *ab*-plane in opposite directions, namely for fields canted towards the $+c^*$ or $-c^*$ axes, respectively). The observed directional anisotropy is related to the uniformly aligned Cl_6 octahedra around the magnetic ion Ru^{3+}.

TT 18.6 Thu 11:30 H7

Evidence for kagome intrinsic excitations in the thermal conductivity of herbertsmithite — •Ralf Claus[1], Jan Bruin[1], Yosuke Matsumoto[1], Masahiko Isobe[1], Jürgen Nuss[1], and Hidenori Takagi[1,2,3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [2]Department of Physics, The University of Tokyo, Bunkyo-ku,Tokyo 133-0022, Japan — [3]Institute for Functional Matter and Quantum Technologies,University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Quantum spin liquids (QSLs) are a novel state of matter that may host exotic excitations like itinerant charge-neutral spin-1/2 quasiparticles (spinons). One prominent candidate for a QSL ground state is the spin-1/2 Heisenberg antiferromagnet on the kagome lattice. Herbertsmithite ($ZnCu_3(OH)_6C_{l2}$) provides a perfect realization of this model. However, despite intense theoretical and experimental efforts the nature of its ground state remains under debate. An important open question concerns the existence of an excitation gap.

To address this issue, we performed thermal transport measurements on herbertsmithite single crystals down to 80 mK. Thermal conductivity (k) only captures mobile excitations in the material and is therefore a powerful tool to detect low-lying (gapless) spinons. In our measurements, we confirmed the absence of a finite k/T(spinon Fermi surface) term but additionally observed an unusual field dependence. By carefully comparing in- and out-of-plane heat flow, we were able to identify kagome intrinsic excitations down to lowest temperature.

TT 18.7 Thu 11:45 H7

Interplay of magnetism and dimerization in pressurized Kitaev compound β-Li_2IrO_3 — •Bin Shen, Anton Jesche, Maximilian Seidler, Friedrich Freund, Philipp Gegenwart, and Alexander A. Tsirlin — EP VI, EKM, University of Augsburg, Germany

Quantum spin liquids in a Kitaev honeycomb model, characterized by their quantum entanglement and fractionalized spin excitations, are subject to extensive studies recently. Here, we present magnetization measurements under pressure for β-Li_2IrO_3, the Kitaev material with the putative pressure-induced spin-liquid state, and construct the temperature-pressure phase diagram. A delicate interplay between magnetism and dimerization is revealed. β-Li_2IrO_3 undergoes incommensurate magnetic ordering at $T_N = 38$ K at ambient pressure. Upon applying hydrostatic pressure, T_N is almost pressure-independent before the transition abruptly disappears at around 1.5 GPa. At around 1.4 GPa, a signature of structural dimerization seen as a small step in the magnetic susceptibility appears at $T_d \approx 120$ K and shifts to higher temperatures upon further compression. Intriguingly, a low-temperature Curie-like upturn with the effective moment of about $0.7\,\mu_B$ is still observed. Using ab initio calculations, we interpret these results as the formation of a partially dimerized state that evades long-range magnetic order but features a fraction of magnetic Ir^{4+} sites.

Work supported by the German Research Foundation through the Sino-German Cooperation Group on Emergent Correlated Matter.

TT 18.8 Thu 12:00 H7

Thermal Transport of a Co-based candidate Kitaev quantum spin liquid (kQSL) material $Na_2Co_2TeO_6$ — •Xiaochen Hong[1,2], Matthias Gillig[1], Richard Hentrich[1], Weiliang Yao[3], Vilmos Kocsis[1], Arthur Witte[1,4], Tino Schreiner[1], Danny Baumann[1], Nicolás Pérez[1], Anja Wolter[1], Yuan Li[3], Bernd Büchner[1,4], and Christian Hess[1,2] — [1]IFW-Dresden, Germany — [2]Bergische Universität Wuppertal, Germany — [3]Peking University, China — [4]TU Dresden, Germany

Motivated by recent theoretical predications that kQSL states can be realized in certain $3d$ transition metal based materials, we studied the thermal transport properties of $Na_2Co_2TeO_6$ single crystals in a wide field-temperature parameter space, up to 16 T and down to 50 mK. We found that phonons, which are strongly scattered by magnetic excitations, are responsible for thermal transport in $Na_2Co_2TeO_6$. By analyzing the field-temperature dependence of the magneto-phonon scattering, we found major similarities between $Na_2Co_2TeO_6$ and the leading kQSL candidate α-$RuCl_3$, supporting theoretical proposals. Besides, we discovered highly anisotropic field effect, signatures of multiple field-induced transitions, and novel oscillation-like thermal transport features. Our findings encourage more studies on $Na_2Co_2TeO_6$, as a promising kQSL material and an exotic quantum magnet.

TT 18.9 Thu 12:15 H7

Spin liquid and ferroelectricity close to a quantum critical point in $PbCuTe_2O_6$ — •Christian Thurn[1], Paul Eibisch[1], Arif Ata[1], Maximilian Winkler[2], Peter Lunkenheimer[2], István Kézsmárki[2], Ulrich Tutsch[1], Yohei Saito[1], Steffi Hartmann[1], Jan Zimmermann[1], Abanoub R. N. Hanna[3,4], A. T. M. Nazmul Islam[4], Shravani Chillal[4], Bella Lake[3,4], Bernd Wolf[1], and Michael Lang[1] — [1]PI, Goethe University Frankfurt — [2]EP V, University Augsburg — [3]IFKP, TU Berlin — [4]HZ Berlin

Geometrical frustration among interacting spins combined with strong quantum fluctuations destabilize long-range magnetic order in favor of more exotic states such as spin liquids (SL). While in quasi-two-dimensional (quasi-2D) systems a number of SL candidates were found, in 3D the situation is less favorable due to reduced quantum fluctuations and more relevant competing states. Here we report studies of thermodynamic, magnetic and dielectric properties on single crystalline and pressed-powder samples of $PbCuTe_2O_6$, a candidate for a 3D frustrated quantum spin liquid (QSL) [1-3] featuring a hyperkagome lattice. Whereas the low-T properties of the powder are consistent with the proposed QSL state [1-3], a more exotic behaviour is found for the single crystals: they show ferroelectric order at $T_{FE} \approx 1$ K, accompanied by strong lattice distortions, and a modified magnetic response − still consistent with a QSL − but with clear indications for quantum critical behaviour.

[1] Koteswararao *et al.*, PRB **90**, 035141 (2014)
[2] Khuntia *et al.*, PRL **116**, 107203 (2016)
[3] Chillal *et al.*, Nat. Commun. **11**, 2348 (2020)

TT 18.10 Thu 12:30 H7

NMR and magnetization investigations of the field-induced order in the frustrated triangular-lattice compound $NaYbSe_2$ — •S. Luther[1,2], K. M. Ranjith[3], T. Reimann[1], Ph. Schlender[4], B. Schmidt[3], J. Sichelschmidt[3], H. Yasuoka[3], J. Wosnitza[1,2], T. Doert[4], M. Baenitz[3], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]MPI for Chemical Physics of Solids, Dresden, Germany — [4]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany

The Yb-based delafossite $NaYbSe_2$ is a triangular-lattice antiferromagnet with space group $R\bar{3}m$. In this compound, spin-orbit coupling leads to a pronounced magnetic anisotropy. The absence of magnetic long-range order at zero field is suggestive for a quantum spin-liquid ground state. From specific-heat and magnetization experiments, magnetically ordered states were observed for $H \perp c$ and $H \parallel c$ exceeding 2 and 9 T, respectively. ^{23}Na ($I = 3/2$) NMR probes the microscopic details of the field-induced magnetic structure. Measurements of the $1/T_1$-relaxation rate are consistent with the specific-heat data. At $H \perp c$ = 5 T, the magnetization indicates an up-up-down spin arrangement with according asymmetric broadening of the NMR spectra. At $H \parallel c$ = 16 T, an umbrella-type configuration of the magnetic moments is predicted, in agreement with a symmetric broadening of the NMR spectra. Low-field measurements reveal a continuous increase of the $1/T_1$-relaxation rate and spectral broadening without any signature of long-range order down to 0.3 K.