TT 26: Correlated Magnetism – Frustrated Systems

Time: Wednesday 9:30–12:45 Location: H33

TT 26.1 Wed 9:30 H33

Temperature-magnetic field phase diagram of the honeycomb Kitaev system $Na_2Co_2TeO_6$ — •Sebastian Erdmann[1], Prashanta Mukharjee[1], Chanhyeon Lee[2], Kwang-Yong Choi[3], and Philipp Gegenwart[1] — [1]Experimental Physics VI, University of Augsburg, Germany — [2]Institute for Materials Research, Tohoku University, Japan — [3]Department of Physics, Sungkyunkwan University, Republic of Korea

Co-based honeycomb magnets have recently attracted considerable interest as promising candidates for the realization of the bond-directional Kitaev exchange [1]. $Na_2Co_2TeO_6$ belongs to this class of materials and displays antiferromagnetic order below 27 K [2]. We investigate a series of phase transitions in $Na_2Co_2TeO_6$ below 4 K, induced by the application of magnetic fields along the a- and a*-axes. The *H-T* phase diagram is determined by low-temperature measurements of the specific heat and magnetic Grüneisen parameter, supplemented by literature results. We also compare the thermodynamic behavior upon field tuning to similar studies on other Kitaev materials, such as the prototype system α-$RuCl_3$.[3]

[1] H. Liu, G. Khaliullin, Phys. Rev. B 97, 014407 (2018).
[2] E. Lefrançois et al., Phys. Rev. B 94, 214416 (2016).
[3] S. Bachus et al., Phys. Rev. B B 103, 054440 (2021).

TT 26.2 Wed 9:45 H33

Anisotropic magnetetoelastic coupling in $Na_3Co_2SbO_6$ — •Prashanta K. Mukharjee[1], Lichen Wang[2], Anton Jesche[1], Julian Kaiser[1], Matthias Hepting[2], Pascal Puphal[2], Masahiko Isobe[2], Bernhard Keimer[2], Philipp Gegenwart[1], and Alexander A. Tsirlin[3] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Max-Planck-Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — [3]Felix Bloch Institute for Solid-State Physics, University of Leipzig, 04103 Leipzig, Germany

Research on 3d-based Co^{2+} materials has intensified as they offer the potential to explore novel regimes of honeycomb magnets, including different versions of the extended Kitaev model. In this study, we investigate the thermodynamic properties of the Kitaev candidate $Na_3Co_2SbO_6$ using complementary thermodynamic measurements, including magnetometry, calorimetry, and high-resolution dilatometry. Our results reveal significant in-plane lattice effects both in the zero-field magnetically ordered phase and in the field-induced states, highlighting a robust anisotropic spin-lattice coupling. Notably, we observe a sign change in both thermal expansion and the structural Grüneisen parameter, which points to a quantum critical endpoint. These findings shed new light on the critical behavior and spin-lattice interactions in $Na_3Co_2SbO_6$ contributing to the understanding of its anisotropic magnetic behaviour.

TT 26.3 Wed 10:00 H33

Revisiting magnetic phases of the Kitaev quantum spin liquid $Na_3Co_2SbO_6$ — •Kranthi Kumar Bestha[1,2], Manaswini Sahoo[1,2], Niccolò Francini[3], Robert Kluge[1], Ryan Christopher Morrow[1], Andrey Maljuk[1], Sabine Wurmehl[1], Sven Luther[4], Hannes Kühne[4], Bernd Büchner[1,2], Laura Teresa Corredor Bohorquez[1], Lukas Janssen[1], and Anja U. B. Wolter[1] — [1]Institute for Solid State Research, Leibniz IFW Dresden 01069, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany — [3]Institute of Theoretical Physics, TU Dresden, 01062 Dresden, Germany — [4]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

The quest for the elusive Kitaev Quantum Spin Liquid phase (KQSL) in Kitaev candidates has resulted in the discovery of unexpected exotic magnetic phases due to competing Kitaev, Heisenberg and off-diagonal interactions in real materials. Honeycomb cobaltate, $Na_3Co_2SbO_6$ (NCSO) has attracted much interest due to the predictions of its proximity to the KQSL phase. Using magnetic and thermodynamic methods, we mapped out the magnetic phase diagram of high-quality NCSO single crystals for all three main crystallographic directions. We observe a $J_{eff} = \frac{1}{2}$ ground state with antiferromagnetic order ($T_N = 7$ K) and multiple field-induced metamagnetic transitions in three field directions. The observed anisotropy and field-induced transitions are modeled within an extended $JK\Gamma\Gamma'$ model. Our work uncovers new exotic magnetic phases both in-plane and out-of-plane field directions.

TT 26.4 Wed 10:15 H33

Magnetic-field induced phase transition crossover in the triangular lattice antiferromagnet $Ba_3CoSb_2O_9$ — •Sanjay Kumar[1], Rashi Nathawat[1], Arvind Kumar Yogi[2], and Satyapal S. Rathore[3] — [1]Functional Ceramics and Smart Materials Lab, Department of Physics, Manipal University Jaipur, Jaipur - 303007, India. — [2]UGC-DAE Consortium for Scientific Research, Indore - 452001, India. — [3]Department of Physics, Cluster University of Jammu, Jammu - 180001, India.

The effect of magnetic field on the ground state properties of triangular lattice antiferromagnet (TLAF) compound $Ba_3CoSb_2O_9$. The temperature-dependent X-ray diffraction (10 to 300 K) shows no structural changes. The temperature and field-dependent susceptibility indicate that TLAF orders antiferromagnetically below $T_N \sim 3$ K. The susceptibility follows a Curie-Weiss law (above 100 K) with q_{CW} = -133.2 K. The frustration index (f $\sim$ 44) indicates a highly frustrated system. Magnetization curves (dM/dH) at 2 K reveal field-induced spin-flop transitions near H $\sim$ 9 T. Magnetic susceptibility shows a broad peak at $T_{max} = 5$ K, becoming more pronounced with increasing field. A spin-glass signature appears near $T_g \sim 6.5$ K but vanishes at higher fields. Interestingly, the magnetic ground state in this compound shows a crossover from the various possible spin orders. A significant shoulder-like hump in heat capacity near $T_c \sim 15$ K suggests structural changes, deviating from the typical λ-anomaly. The change in magnetic properties is attributed to the interplay between antisite defects, quantum fluctuations, and geometric frustration in TLAF.

TT 26.5 Wed 10:30 H33

First-principles modeling of Ni-based honeycomb compounds — •Thore Martens and Alexander Tsirlin — Leipzig University, Germany

In recent years, there has been an increasing interest in Kitaev materials for spins higher than 1/2. Using Density functional theory (DFT), anisotropic spin couplings as well as single-ion anisotropy are calculated and compared for several Ni-based honeycomb compounds: $KNiAsO_4$, $BaNi_2(AsO_4)_2$, $BaNi_2(PO_4)_2$ and $Na_3Ni_2BiO_6$. Most of these investigated compounds share a particularly large antiferromagnetic J_3 and a weaker ferromagnetic J_1 as leading couplings giving rise to a zig-zag magnetic structure. The dependence of these couplings on U from LSDA+U as well as full calculations on the tensor elements of J_1 are performed. From this, potential Kitaev interactions are obtained for the four Ni-compounds.

TT 26.6 Wed 10:45 H33

Exploring Geometrical Frustration in Ho_3ScO_6-II: Magnetic Properties and Structural Insights — •Abanoub Hanna[1], Cintli Aguilar Maldonado[1], and Bella Lake[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Platz 1, D-14109 Berlin, Germany — [2]Institut für Festkörperphysik,Technische Universität Berlin, Berlin, Germany

Geometrical frustration occurs in magnetic compounds when the arrangement of magnetic ions in triangular or tetrahedral lattices leads to competing interactions, resulting in non-classical magnetic states. This study examines the cubic compound Ho_3ScO_6-II, which crystallizes in a bixbyite-type structure with a centrosymmetric cubic space group Ia3* and exhibits no magnetic ordering above 1.8 K, underscoring its geometrically frustrated nature. Unlike its polymorph Ho_3ScO_6-I, which shows long-range magnetic order at 4.4 K, Ho_3ScO_6-II lacks magnetic anisotropy and presents a Curie-Weiss temperature of approximately -20 K and an effective magnetic moment (μ_{eff}) of 9.8 μB, indicating significant antiferromagnetic interactions. Additionally, the study compares Ho_3ScO_6-II with Er_3ScO_6, which is isostructural and exhibits magnetic ordering around 2.1 K that is suppressed under external magnetic fields. This comparison highlights the contrasting behaviours of these compounds, contributing to a deeper understanding of frustrated magnetism within the RE_3ScO_6 system (RE = Ho, Er). The findings provide valuable insights into the unique structural and magnetic properties of Ho_3ScO_6-II and suggest potential applications in spintronic devices and quantum computing.

15 min. break

TT 26.7 Wed 11:15 H33

Continuous Similarity Transformations for the Easy-Axis XXZ Model on the Honeycomb Lattice — •Matthias R. Walther[1], Dag-Björn Hering[2], Vanessa Sulaiman[2], Maximilian Bayer[1], Götz S. Uhrig[2], and Kai P. Schmidt[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany — [2]Condensed Matter Theory, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany

Neutron scattering experiments on $YbCl_3$ show that it realizes the antiferromagnetic Heisenberg model on a honeycomb lattice [1]. While key features are captured by linear spin-wave theory (LSWT), a full dispersion cannot be reproduced. We apply continuous similarity transformations (CSTs) [2-4] to the easy-axis antiferromagnetic XXZ-model on the honeycomb lattice. This allows us to derive an effective model which takes the relevant magnon-magnon interactions beyond LSWT into account targeting a quantitative description of the single-particle properties. The CST flow equations are truncated in momentum space by the scaling dimension d so that all contributions with $d \leq 2$ are taken into account. The resulting quartic magnon-conserving effective Hamiltonian is analyzed in the zero-, one-, and two-magnon sector.

[1] G. Sala et al., Nat. Comm. 12, 171 (2021).
[2] M.R. Walther et al., Phys. Rev. Res., 013132 (2023).
[3] M. Powalski et al., Rev. Lett. 115, 207202 (2015).
[4] M. Powalski et al., SciPost Phys. 4, 001 (2018).

TT 26.8 Wed 11:30 H33

Magnetic Frustration and Weak Mn Magnetic Ordering in $EuMn_2P_2$ — Sarah Krebber[1], Marvin Kopp[1], Jens Müller[1], Jörg Sichelschmidt[2], Michael Baenitz[2], Kurt Kummer[3], Cornelius Krellner[1], and •Kristin Kliemt[1] — [1]Physikalische Institut, Goethe Universität Frankfurt, Deutschland — [2]Max-Planck-Insitut für Chemische Physik fester Stoffe, 01187 Dresden, Deutschland — [3]European Synchrotron Radiation Facility, 38043 Grenoble, France

$EuMn_2P_2$ is a member of the Eu-based 122-systems with a trigonal $CaAl_2Si_2$ crystal structure. The magnetic properties of the Eu ion in this compound are located in triangular layers of Eu^{2+}. Several quantaties indicated the presence of A-type antiferromagnetic Eu order at $\approx 18\,\mathrm{K}$, with magnetic moments oriented in the a-a plane. Nevertheless, no magnetic order of Mn was observed [1,2]. This is intriguing, given that the analogous compounds $EuMn_2As_2$ and $EuMn_2Sb_2$ exhibit phase transitions attributed to Mn magnetic order at elevated temperatures ($T_N = 135$ K, $T_N = 128$ K) [3,4].

In this study, we present the results of electron spin resonance (ESR), heat capacity, magnetization, nuclear magnetic resonance (NMR) and electrical resistivity measurements on $EuMn_2P_2$ single crystals, which exhibite a weak magnetic ordering attributed to Mn magnetism.

[1] A. Payne et al., J. Solid State Chem. 163, 2 (2002);
[2] T. Berry et al., J. Am. Chem. Soc. 145, 8 (2023);
[3] V. K. Anand et al., Phys. Rev. B 94, 014431 (2016);
[4] I. Schellenberg et al., ZAAC 636, 85 (2010).

TT 26.9 Wed 11:45 H33

Exploring the Anisotropic Shastry-Sutherland Model by Strain Tuning of $SrCu_2(BO_3)_2$ — •Francisco Lieberich[1,4], Pascal Puphal[2], Ekaterina Pomjakushina[3], and Elena Gati[1,4] — [1]MPI-CPfS, Dresden, Germany — [2]MPI-FKF, Stuttgart, Germany — [3]PSI, Villigen, Switzerland — [4]TUD, Dresden, Germany

The Shastry-Sutherland model is a hallmark of frustrated magnetism and is realized by $SrCu_2(BO_3)_2$, where competing intra-dimer and inter-dimer interactions J and J' stabilize a dimerized ground state. The Shastry-Sutherland model can be generalized to an anisotropic model with two sets of inequivalent couplings J_1, J_2 and J_1', J_2'. This model is predicted to host novel ground states [1] and may address the debate [2] on the nature of the plaquette phase of $SrCu_2(BO_3)_2$. Experimentally, anisotropic strains break the lattice symmetry of $SrCu_2(BO_3)_2$ and may therefore be used to tune the anisotropy in the Shastry-Sutherland model. We use the AC elastocaloric effect, a thermodynamic probe of strain-tuned quantum materials [3], to map out the entropic landscape of $SrCu_2(BO_3)_2$ under large anistropic strains. By comparing the results under [100] and [110] strain, we disentangle the effects of symmetry-breaking and symmetry-conserving strains on $SrCu_2(BO_3)_2$. Our phase diagrams reveal features consistent with hydrostatic-pressure studies [4], alongside new effects that may arise from symmetry breaking.

Supported by the DFG through SFB 1143.

[1] Boos et al., PRB 100, 140413(R) (2019);
[2] Zayed et al., Nat. Phys. 13, 962 (2017);
[3] Ikeda et al., RSI 90, 083902 (2019);
[4] Guo et al., PRL 124, 206602 (2020).

TT 26.10 Wed 12:00 H33

Search for Precursors of Multi-Magnon Bound States in Li_2CuO_2 Single Crystals in Specific Heat Data — •Stefan-Ludwig Drechsler[1], Eli Zoghlin[2], Wolfram Lorenz[1], and Ulrich Roessler[1] — [1]IFW-Dresden, Dresden, Germany — [2]J. Hopkins University, Baltimore, Maryland, USA

We report specific heat c_p-data for high quality single crystals of the edge-sharing chain cuprate Li_2CuO_2 collected in a wide temperature region from 20 to 70 K well above the Ne'el transition $T_N \approx 9.2$ to 9.4 K at ambient magnetic field. The c_p is analyzed within a sensitive c_p/T^3-plot adopting and generalizing an analytical expression [1] by adding precursor multi-magnon bound state (PMMBS) of any order. This way, the problem of missing intensity around 40 K can be resolved. The obtained excitation energies of PMMBS are in accord with recent inelastic neutron scattering data for Li_2CuO_2 [2] regarding single-magnon, two-magnon and three-magnon bound states. The results are discussed within the context of a recenly proposed Bose condensation scenario of MMBS [3] at very low temperature and ambient field.

[1] S. Ebisu *et al.*, J. Phys.Chem.Sol. **59**, 1407 (1998);
[2] E. Zoghlin *et al.*, PRB **108** 064408 (2023);
[3] C.E. Agrapidis, S.-L. Drechsler, S. Nishimoto, arXiv: 2410.00734, Phys. Rev. X (submitted).

TT 26.11 Wed 12:15 H33

Anisotropic Spin Ice on a Breathing Pyrochlore Lattice — •Gloria Isbrandt[1,2], Frank Pollmann[1,2], and Michael Knap[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

Spin ice systems have long captivated researchers due to their exotic magnetic properties and emergent excitations. Recently, breathing pyrochlore compounds have been identified as a platform for studying novel phases, including fracton physics and quantum spin liquids. We explore a spin ice model on a breathing pyrochlore lattice, introducing sublattice-dependent anisotropic interactions that are potentially realizable experimentally, for example, through uniaxial strain. We theoretically uncover a rich phase diagram by varying the strain and show how these anisotropic constraints reduce the ground state degeneracy across the different phases. Our numerical simulations reveal that, at low temperatures, the models undergo a crossover into a constrained spin ice manifold, characterized by an entropy density that falls below the celebrated Pauling entropy of conventional spin ice. Moreover, we observe glassy dynamics in spin correlations when probing the out-of-equilibrium behavior, suggesting slow relaxation and memory effects. This model provides a new perspective on spin ice physics, offering a potentially robust platform for studying fracton phenomena and experimental exploration of constrained magnetism and emergent glassy dynamics.

TT 26.12 Wed 12:30 H33

Efficient Optimization and Conceptual Barriers with Projected Entangled-Pair States — •Erik Weerda[1], Daniel Alcalde[1,2], Konrad Schröder[1], and Matteo Rizzi[1,2] — [1]University of Cologne, Cologne, Germany — [2]Forschungszentrum Jülich

Finite projected entangled-pair states (PEPS) are becoming a widely used tool in the computational study of strongly correlated systems. However, no standard set of computational tools has yet emerged to exploit the power of this approach. In this work we investigate a promising approach to ground state search with PEPS based on sampling methods. Along with presenting strategies for more effi cient optimisation, we also discuss conceptual barriers associated with this approach. A benchmark illustrates the power of these tools in the study of ground states of frustrated magnetic models.