TT 49: Frustrated Magnets: Strong Spin-Orbit Coupling I

Time: Wednesday 15:00–18:15 Location: H 2053

TT 49.1 Wed 15:00 H 2053

Two-dimensional optical spectroscopy of a Kitaev magnet — •Wolfram Brenig[1] and Olesia Krupnitska[1,2] — [1]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany — [2]Institute for Condensed Matter Physics, NASU, Svientsitskii Str. 1, 79011 Lviv, Ukraine

We study electric field induced second order two-dimensional spectroscopy (2DS) in a Kitaev magnet. This frustrated magnet hosts a quantum spin-liquid, featuring fractionalization in terms of mobile Majorana fermion and static $\mathbb{Z}_2$ flux-vison elementary excitations. We show that finite temperature 2DS does not only probe characteristic features of both fractional excitations, but also and depending on the directions analyzed within the two-dimensional frequency plane, allows to extract single quasiparticle lifetimes from the multi-particle continua of the 2DS response functions. These properties will be discussed both, in the homogeneous flux state at low temperatures, as well as in the random flux state at elevated and up to high temperatures. At the flux proliferation crossover, we suggest an interpolation between these two temperature regimes.
Work profited from interaction with Roser Valentí, Marius Möller and David Kaib.

TT 49.2 Wed 15:15 H 2053

Bond disorder in extended Kitaev-Heisenberg models — •Georgia Fragkopoulou and Matthias Vojta — Technische Universität Dresden

We study the effect of bond disorder in extended Kitaev-Heisenberg models on the honeycomb lattice, relevant for materials such as α-$RuCl_3$, in the semiclassical limit using a combination of T-matrix and real-space spin-wave approaches. Focussing on the regime of large applied magnetic field, we discuss two distinct but related disorder-induced phenomena, namely spin textures and in-gap states. Depending on whether the impurity and the field direction break the discrete lattice symmetries, impurity-induced textures either arise at arbitrary field and impurity strength and without spontaneous symmetry breaking, or they only occur beyond a certain impurity strength and are accompanied by spontaneous symmetry breaking. The latter can be understood precursors of a low-field ordered phase and induce magnetic states below the bulk gap. A finite impurity concentration turns these isolated states into impurity bands. As a result, there is a large field regime above the bulk transition to the high-field state where impurity-induced states fill the bulk spin gap. We illustrate the field dependence of these in-gap states for parameters relevant for α-$RuCl_3$, and we connect our results to heat-transport and NMR data which indicated their presence.

TT 49.3 Wed 15:30 H 2053

Finite-size effects in Heisenberg-Kitaev models — •Wilhelm Krüger and Lukas Janssen — Institute for Theoretical Physics, TU Dresden, 01062 Dresden

The Heisenberg-Kitaev model is a paradigmatic model to describe the magnetism in honeycomb-lattice Mott insulators with strong spin-orbit coupling, such as A_2IrO_3 ($A = \mathrm{Na, Li}$), α-$RuCl_3$, and $Na_2Co_2TeO_6$. Due to the sign problem in quantum Monte Carlo simulations, the model can be studied numerically exactly only on small lattices. Here, we investigate in detail the finite-size effects, by carefully comparing numerical exact diagonalization calculations with semi-analytical nonlinear spin-wave theory. This allows us to establish a protocol to obtain improved estimates for various observables from finite-size extrapolations to the thermodynamic limit, including the spectral gap, the local magnetization, and phase transition points.

TT 49.4 Wed 15:45 H 2053

Spin-Peierls Kitaev-Heisenberg models: auxiliary field quantum Monte Carlo studies — Toshihiro Sato[1], •João Carvalho-Inacio[2], Jeroen van den Brink[1], and Fakher F. Assaad[2] — [1]IFW Dresden — [2]University of Würzburg

Recently we have formulated auxiliary field quantum Monte Carlo simulations Heisenberg-Kitaev model [1]. This approach offers the possibility of reaching temperature scales roughly a factor two smaller that the magnetic scale before running into severe negative sign problems. Here we show that we can generalize this approach to include Einstein phonons. Importantly we show that the inclusion of phonons does not render the sign problem more severe such that the approach offers the possibility of investigating signatures of fractionalization on phonon spectral functions.
[1] T. Sato, F. F. Assaad, Phys. Rev. B 104 (2021) L081106.

TT 49.5 Wed 16:00 H 2053

Spin vestigial orders in extended Heisenberg-Kitaev models near hidden SU(2) points: Application to $Na_2Co_2TeO_6$ — •Niccolò Francini and Lukas Janssen — Technische Universität Dresden, Dresden, Germany

The honeycomb magnet $Na_2Co_2TeO_6$ has recently been argued to realize an approximate hidden SU(2) symmetry that can be understood by means of a duality transformation. Using classical Monte Carlo simulations, we study the finite-temperature phase diagram of the Heisenberg-Kitaev-Γ-Γ' model near the hidden-SU(2)-symmetric point, in the presence of a six-spin ring exchange perturbation. At low temperatures, the model features collinear single-$\mathbf{q}$ zigzag and noncollinear triple-$\mathbf{q}$ ground states, depending on the sign of the ring exchange coupling. In the vicinity of the hidden-SU(2)-symmetric point, the magnetic long-range orders melt in two stages. The two phases at intermediate temperatures spontaneously break spin rotational and lattice translational symmetries, respectively, leaving time reversal symmetry intact, and are understood as vestigial orders of the underlying magnetic states. We identify these vestigial orders as $\mathbb{Z}_3$ spin nematic and $\mathbb{Z}_4$ spin current density wave phases. The latter is a candidate for the paramagnetic 2D long-range-ordered state observed in $Na_2Co_2TeO_6$.

TT 49.6 Wed 16:15 H 2053

Magnetic ground state of the Kitaev material $Na_2Co_2TeO_6$ — Wilhelm G. F. Krüger, Niccolò Francini, and •Lukas Janssen — TU Dresden, Dresden, Germany

Among the candidate Kitaev materials, the honeycomb Mott insulator $Na_2Co_2TeO_6$ has received significant recent attention. The nature of its magnetic ground state, however, has been a matter of considerable debate. We reveal an unusually high symmetry in the single-crystal neutron scattering spectrum that is inconsistent with a zigzag ground state and instead indicates a noncoplanar triple-$\mathbf{q}$ magnetic ordering. Implications concerning the proximity of $Na_2Co_2TeO_6$ to the Kitaev quantum spin liquid will be pointed out as well.
[1] W. G. F. Krüger, W. Chen, X. Jin, Y. Li, L. Janssen, Phys. Rev. Lett. **131** (2023) 146702
[2] N. Francini, L. Janssen, arXiv:2311.08475

15 min. break

TT 49.7 Wed 16:45 H 2053

Field and polarization dependent quantum spin dynamics in the honeycomb magnet $Na_2Co_2TeO_6$: Magnetic excitations and continuum — •Patrick Pilch[1], Laur Peedu[2], Anup Kumar Bera[3], Seikh Mohammad Yusuf[3,4], Urmas Nagel[2], Toomas Rõõm[2], and Zhe Wang[1] — [1]Department of Physics, TU Dortmund University, Dortmund, Germany — [2]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia — [3]Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, India — [4]Homi Bhabha National Institute, Anushaktinagar, Mumbai, India

We report terahertz spectroscopic measurements of quantum spin dynamics in the spin-1/2 honeycomb magnet $Na_2Co_2TeO_6$ as a function of applied magnetic field with different terahertz polarizations [1]. Distinct field dependencies of the resolved spin dynamics are identified in three regimes, which are separated by two critical fields at $B_{c1} \approx 7$ and $B_{c2} \approx 10$ T. A polarization selective continuum is observed in the intermediate phase, featuring spin fluctuations of a proximate quantum spin liquid.
[1] Pilch et al., Phys. Rev. B 108, L140406 (2023)

TT 49.8 Wed 17:00 H 2053

Rotational disorder in the triangular spin-liquid candidate $Na_2BaCo(PO_4)_2$ — Vera P. Bader[1], Ivo Heinmaa[2], Raivo Stern[2], Felix Schilberth[3], Joachim Deisenhofer[3], Istvan Kézsmárki[3], Philipp Gegenwart[1], and •Alexander A. Tsirlin[1,4]

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Using high-resolution x-ray diffraction, nuclear magnetic resonance, and infrared spectroscopy, we resolve the previously overlooked ferro-rotational distortion in the spin-$\frac{1}{2}$ triangular antiferromagnet $Na_2BaCo(PO_4)_2$. Cooperative rotations of the CoO_6 octahedra reduce the symmetry to $P\bar{3}$ while leading to only minor changes in the spin Hamiltonian. The rotations are accompanied by Na displacements that indicate an inherent structural randomness, which is present even at low temperatures and increases on heating. Our *ab initio* molecular dynamics simulations suggest that Na disorder is intimately linked to the cooperative rotations. We propose two mechanisms that may lead to the suppression of magnetic order in $Na_2BaCo(PO_4)_2$ due to structural randomness and elucidate the unusually low Néel temperature ($T_N/J \simeq 0.1$) of this material. Our results suggest the importance of lattice degrees of freedom and hidden randomness for the physics of spin-liquid candidates.

TT 49.9 Wed 17:15 H 2053

Understanding the Magnetic Behavior of $CoNb_2O_6$: Insights from Ab Initio Modeling — •Amanda Konieczna[1], Stephen M. Winter[2], and Roser Valentí[1] — [1]Goethe University Frankfurt — [2]Wake Forest University

The quasi-one-dimensional Ising-like system $CoNb_2O_6$ has been a subject of intense investigation, particularly regarding its microscopic model and the potential role of Kitaev interactions. Despite various experiments, the system's magnetic behavior remains a topic of debate with different suggestions arising [1,2]. We employ an ab initio-based model to investigate $CoNb_2O_6$'s magnetism. The approach involves the modeling of an ab-initio derived Hubbard Hamiltonian and utilizing projective diagonalization techniques to construct a Spin Hamiltonian. This presentation discusses the results of our theoretical modeling approach in the context of experimental observations to give further insights into $CoNb_2O_6$'s magnetic behavior.

[1] Coldea *et al.*, Phys. Rev. B **108** (2023) 184417
[2] Armitage *et al.*, Nat. Phys. **17** (2021) 832

TT 49.10 Wed 17:30 H 2053

Understanding the Hamiltonian of α-RuCl$_3$ through Non-Linear Spin-Wave Analysis — Jonas Habel[1,2], Roderich Moessner[3], and •Johannes Knolle[1,2,4] — [1]Technical University of Munich, Germany — [2]Munich Center for Quantum Science and Technology, Germany — [3]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [4]Blackett Laboratory London, UK

α-RuCl$_3$ has attracted much attention recently due to its potential to host a Kitaev spin liquid at intermediate magnetic fields, whose stability crucially depends on the model Hamiltonian and its parameters. These parameters are commonly probed by performing inelastic neutron scattering (INS) in the high-field limit, where the magnetic moments are fully polarized and spin-wave excitations are well-defined, and subsequently fitting the observed INS intensity to a theoretical linear spin-wave prediction. However, experimental estimates vary widely, in particular for the Kitaev interaction, which is vital for a spin liquid phase. Our work aims to improve these estimates by incorporating non-linear spin-wave effects in the theoretical computations. Concretely, we investigate neutron scattering data for a three-dimensional multi-layer of α-RuCl$_3$ using an augmented Kitaev-Heisenberg model. Preliminary results show that non-linear quantum interactions have a significant impact on the spin-wave spectrum and should not be neglected when fitting model parameters to INS data.

TT 49.11 Wed 17:45 H 2053

The role of phonons in the thermal Hall effect of α-RuCl$_3$ — •Ralf Claus, Jan Bruin, Yosuke Matsumoto, and Hidenori Takagi — Max-Planck-Institut für Festkörperforschung, Stuttgart 70569, Deutschland

The observation of a half-integer quantized plateau in the thermal Hall conductivity κ_{xy} of the Kitaev quantum spin liquid candidate α-RuCl$_3$ was interpreted as evidence for a topological Majorana edge mode [1]. Recently, additional studies of κ_{xy} were performed [2], including those offering different explanations for the possible heat carrying particles such as topological magnons [3] and phonons [4]. To narrow down the nature of these itinerant quasiparticles, we performed a comprehensive study of the thermal Hall angle $\tan(\theta) = \kappa_{xy}/\kappa_{xx}$ on samples grown using CVT and Bridgman techniques. Surprisingly, we find that $\tan(\theta)$ is fairly similar among different samples despite large differences in the longitudinal thermal conductivity κ_{xx}. This scaling suggests a substantial role of phonons and puts constraints on the Majorana or topological magnon scenarios. Furthermore, we propose a mechanism involving phonon drag, which would explain the dependence of the Hall amplitude on the longitudinal phonon conductivity.

[1] Kasahara et al., Nature 559 (2018) 227
[2] Bruin, Claus et al., Nat. Phys. 18 (2022) 401
[3] Czajka et al., Nat. Mater. 22 (2023) 36
[4] Lefrançois et al., Phys. Rev. X 12 (2022) 021025

TT 49.12 Wed 18:00 H 2053

β-RuCl$_3$ / graphene heterostructures: a new playground for exotic physics — •Aleksandar Razpopov, Sananda Biswas, and Roser Valentí — Institut für Theoretische Physik, Goethe Universität, Frankfurt, Germany

In recent years emerging novel phases in α-RuCl$_3$-graphene heterostructures have been intensively discussed [1-4] in the context of Kitaev physics and its charge transfer properties. In contrast, β-RuCl$_3$, a polymorph of α-RuCl$_3$, has received much less attention. This system has a chain-like structure of Ru ions instead of the honeycomb lattice pattern in α-RuCl$_3$. Recently, 1D-heterostructures of β-RuCl$_3$ on graphene have been fabricated in the form of high quality uniform and long-single crystalline atomic scale wires [5]. In this talk, we will present a first principles study of the electronic structure of β-RuCl$_3$/graphene heterostructures and will discuss the importance of strain effects to control charge transfer between these two compounds and its relevance for the resulting electronic properties.

[1] Rossi et al., Nano Lett. 23, 17, 8000
[2] Balgley et al., 22, 10, 4124
[3] Biswas et al., Phys. Rev. Lett. 123, 237201
[4] V. Leeb et al., Phys. Rev. Lett. 126, 097201
[5] Tomoya et al., Adv. 9, eabq5561