# TT 8: Frustrated Magnets – Strong Spin-Orbit Coupling

Time: Monday 17:15–19:00 Location: H10

TT 8.1 Mon 17:15 H10

**$\alpha$-RuCl$_3$ probed by ultrasound under hydrostatic pressure** — •Andreas Hauspurg[1,2], S. Zherlitsyn[1], T. Helm[1], T. Yanagisawa[3], V. Tsurkan[4], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Department of Physics, Hokkaido University, Sapporo, Japan — [4]Institute of Physics, University of Augsburg, Germany

As a prime candidate for a quantum spin liquid (QSL) in the frame of the Kitaev model, is the honeycomb material $\alpha$-RuCl$_3$ of particular interest. Although $\alpha$-RuCl$_3$ exhibits antiferromagnetic order below 7 K, it is considered as proximate to the QSL. The QSL features fractionalized quasiparticle excitations. A promising approach to investigate such excitations is to study the coupling between fractionalized quasiparticles and phonons. This affects the attenuation coefficient and the sound velocity of ultrasound. Our recent studies of the elastic properties of $\alpha$-RuCl$_3$ show a promising path to unveil the unconventional physics of the debated QSL phase. Here, we present low-temperature results of the sound velocity and attenuation in external magnetic fields and under hydrostatic pressures. The observed anomalies in the acoustic properties and strong magnetoelastic couplings shed new light on the unconventional physics in this compound. At a pressure of 11.3 kbar the antiferromagnetic order is completely suppressed.

TT 8.2 Mon 17:30 H10

**Fractional Excitation-induced Phonon Renormalization in $\alpha$-RuCl$_3$** — •Adrian Merritt[1], Xiao Wang[1], Alexei Bosak[2], Luigi Paolasini[2], Alexandre Ivanov[3], Rolf Heid[4], and Yixi Su[1] — [1]Jülich Centre for Neutron Science JCNS-FRM II, Forschungszentrum Jülich GmbH, Garching, Germany — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [3]Institut Laue-Langevin, Grenoble, France — [4]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Karlsruhe, Germany

The quantum spin liquid (QSL) phase is of immense interest to condensed matter physicists, and have been studied for decades. With a Kitaev model that is exactly solvable and gives a QSL ground state, more recent work has focused on the $J_{eff}$=1/2 materials and in particular, $\alpha$-RuCl$_3$. Above the critical magnetic field $B_c$ 7T and below T 6K there is evidence for the half-integer quantized plateau possibly arising from the fractional excitations in the QSL phase. Recent theoretical work has shown that the fractional excitations can induce phonon renormalization via the spin-lattice coupling, and would in particular affect the acoustic phonons near the zone boundary. Our measurements have focused on the phonon dispersion in $\alpha$-RuCl$_3$ to observe this phonon renormalization effect in the putative QSL phase. We have been able to survey the acoustic phonons in the relevant scattering directions under magnetic fields using single crystals. We will discuss our results with a focus on examining the low-energy acoustic phonon branches we measured in comparison to published work as well as the observed phonon renormalization effect.

TT 8.3 Mon 17:45 H10

**Quantum Monte Carlo simulations of generalized Kitaev models: applications to** $\alpha$-RuCl$_3$ — •Toshihiro Sato[1] and Fakher F. Assaad[1,2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Germany

We introduce a phase pinning approach in the realm of the auxiliary field quantum Monte Carlo (QMC) algorithm that mitigates the severity of the negative sign problem inherent to QMC methods of frustrated spin systems [1]. This allows us to access high-temperature thermodynamic and dynamical properties of the aforementioned systems and, for instance, carry out exact QMC simulations in a window of temperatures relevant to experiments for various frustrated magnets. We use our method to carry out extensive simulations of thermodynamic properties under magnetic fields in generalized Kitaev models describing $\alpha$-RuCl$_3$, and discuss the characteristic feature in the field-direction dependence of the magnetic susceptibility, the specific heat as well as the magnetotropic coefficient. Our numerical results allow for direct comparison with recent measurements of the magnetotropic coefficient in $\alpha$-RuCl$_3$ [2].

[1] T. Sato and F. F. Assaad, Phys. Rev. B. 104, L081106 (2021)
[2] K. A. Modic et al., Nat. Phys. (2020)

TT 8.4 Mon 18:00 H10

**RuCl$_3$: Phonon (Hall) transport and sibling compounds RuBr$_3$, RuI$_3$** — •David A S Kaib[1], Sananda Biswas[1], Stephen M Winter[2], Kira Riedl[1], Aleksandar Razpopov[1], Ying Li[3], Steffen Backes[4], Igor I Mazin[5], and Roser Valenti[1] — [1]Goethe-Universität, Frankfurt, Germany — [2]Wake Forest University, Winston-Salem, NC 27109, USA — [3]School of Physics, Xi'an Jiaotong University, Xi'an 710049, China — [4]Institut Polytechnique de Paris, Route de Saclay, 91128 Palaiseau, France — [5]George Mason University, Fairfax, VA 22030, USA

We present results of two studies related to the Kitaev candidate material RuCl$_3$:

Recent experimental studies have pointed to the presence of significant magnetoelastic coupling in RuCl$_3$ and have highlighted unusual thermal transport signatures under magnetic field. We compute the pseudospin-phonon coupling in RuCl$_3$ from first principles and use it to model the intrinsic thermal transport from phonons scattered by spin fluctuations. This includes both the longitudinal as well as the transversal (Hall) conductivity.

In the second part of the talk, we analyze two new sibling compounds to RuCl$_3$: RuBr$_3$ and RuI$_3$. While current samples show a bad metal behavior in RuI$_3$, our first principles calculations predict a Mott insulator close to the Mott-metal transition in the pristine parent compound, with a dominant Kitaev interaction and negligible Heisenberg exchange.

TT 8.5 Mon 18:15 H10

**High-field ESR studies of the cubic Iridium hexahalide compounds $(NH_4)_2IrCl_6$ and $K_2IrCl_6$** — •Lakshmi Bhaskaran[1], Alexey N. Ponomaryov[2], Jochen Wosnitza[1,3], Nazir Khan[4], Alexander A. Tsirlin[4], Mike E. Zhitomirsky[5], and Sergei A. Zvyagin[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL) and Würzburg-Dresden Cluster of Excellence ct.qmat, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Institut für Festkörper- und Materialphysik, TU Dresden, Dresden, Germany — [4]University of Augsburg, Augsburg, Germany — [5]University Grenoble Alpes, Grenoble, France

We report on high-field electron spin resonance studies of two iridium hexahalide compounds, $(NH_4)_2IrCl_6$ and $K_2IrCl_6$ [1]. In the paramagnetic state, our measurements reveal isotropic $g$-factors $g = 1.79(1)$ for the $Ir^{4+}$ ions, in agreement with their cubic symmetries. Most importantly, in the magnetically ordered state, we observe two magnon modes with zero-field gaps of 11.3 and 14.2 K for $(NH_4)_2IrCl_6$ and $K_2IrCl_6$, respectively. Based on that and using linear spin-wave theory, we estimate the nearest-neighbor exchange couplings and anisotropic Kitaev interactions, $J_1/k_B = 10.3$ K, $K/k_B = 0.7$ K for $(NH_4)_2IrCl_6$, and $J_1/k_B = 13.8$ K, $K/k_B = 0.9$ K for $K_2IrCl_6$, revealing the nearest-neighbor Heisenberg coupling as the leading interaction term, with only a weak Kitaev anisotropy.

[1] L. Bhaskaran et al., Phys. Rev. B **104**, 184404 (2021).

TT 8.6 Mon 18:30 H10

**Spin-orbit excitons in the $j_{\rm eff}$=1/2 compound $K_2IrCl_6$** — •Philipp Warzanowski[1], Marco Magnaterra[1], Karolin Hopfer[1], Christoph Sahle[2], Marco Morreti Sala[3], Giulio Monaco[4], Petra Becker[5], Ladislav Bohatý[5], and Markus Grüninger[1] — [1]Inst. of Physics II, University of Cologne — [2]European Synchrotron Radiation Facility, Grenoble Cedex, France — [3]Dip. di Fisica, Politecnico di Milano, Italy — [4]Dip. di Fisica e Astronomia, Università di Padova, Italy — [5]Sect. Crystallography, Inst. of Geology and Mineralogy, University of Cologne

Spin-orbit entangled Mott insulators offer new playgrounds to explore novel ground states. Iridates with a $t_{2g}^5$ electron configuration are popular platforms to realize $j_{\rm eff}$ =1/2 systems due to the large cubic crystal field and strong spin-orbit coupling. Spectroscopies, RIXS in particular, show that thus far all iridates harbour non-cubic crystal field distortions, which turn the ground state away from an ideal $j_{\rm eff}$ = 1/2 state. In this context, the (globally) cubic compound $K_2IrCl_6$ is a promising candidate to host ideal $j_{\rm eff}$ = 1/2 moments. However, both RIXS and infrared spectroscopy show a splitting of the spin-orbit exciton. Within a single-site scenario, we extract a spin-orbit coupling $\lambda = 435$ meV and a non-cubic crystal field $\Delta = 60$ meV, yielding a ground state of 99.8% $j_{\mathrm{eff}} = 1/2$ character. To explore the origin of non-cubic distortions, we discuss the possible effects of i) librations [1], ii) the coupling to phonons, and iii) defects [2].

[1] N. Khan *et al.*, Phys Rev B **103**, 125158 (2021)
[2] S.-S. Bao *et al.*, Inorg. Chem. **57**, 13252 (2018)

TT 8.7 Mon 18:45 H10

**Fragility of charge frustration in high-pressure $CsW_2O_6$** — •Pascal Reiss[1], Masahiko Isobe[1], and Hidenori Takagi[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Department of Physics, The University of Tokyo, Bunkyo, Tokyo, Japan

The transition metal compound $CsW_2O_6$ represents an intriguing example of a pyrochlore structure at quarter filling. Starting from a nominal $W^{5.5+}$ oxidation state, the system suffers a metal-to-insulator transition around $T_c \approx 215$ K where a breathing distortion leads to the formation of regular molecular $W_3$ trimers with 2 localised electrons each, and a remaining $W^{6+}$ site devoid of $5d$ electrons [1]. Recently, it was proposed that in this low-temperature phase, the interplay between a strong spin-orbital coupling and the transfer integral could realise a rare case of an intrinsically half-filled flat band dispersion with a stiff spin chirality [2].

In this talk, we will present our recent high pressures transport measurement on $CsW_2O_6$. With increasing pressure, we find that the low-temperature insulating phase is stabilised as the metal-to-insulator transition shifts to higher temperatures. We will discuss our results in the light of recent theoretical proposals.

[1] Y. Okamoto et al., Nat. Commun. 11 (2020)
[2] N. Nakai and C. Hotta, Nat. Commun. 13 (2022)