## MA 22: Frustrated Magnets - Spin Liquids 1 (joint session TT/MA)

Time: Tuesday 9:30–13:00

MA 22.1 Tue 9:30 HSZ 304

Low temperature thermal transport studies on the kagome quantum spin liquid candidate herbertsmithite — JAN BRUIN, •RALF CLAUS, YOSUKE MATSUMOTO, JÜRGEN NUSS, MASAHIKO ISOBE, and HIDENORI TAKAGI — Max Planck Institute for Solid State Research, 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). The prototype for a QSL ground state is the spin-1/2 Heisenberg antiferromagnet on the kagome lattice. In terms of materials, herbertsmithite (ZnCu<sub>3</sub>(OH)<sub>6</sub>C<sub>12</sub>) provides a perfect realization of this model. However, despite theoretical and experimental efforts the nature of its ground state remains under debate. An important question concerns the existence of an excitation gap.

To address this issue, we performed thermal transport measurements down to 80 mK. The measurement of the 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) term but observed a robust T-squared power-law behavior. I will discuss the possible QSL ground state scenarios in detail as well as an unusual field dependence.

MA 22.2 Tue 9:45 HSZ 304

Magnetic properties of the NaYbO<sub>2</sub> and KYbO<sub>2</sub> triangular antiferromagnets — •FRANZISKA GRUSSLER, SEBASTIAN BACHUS, PHILIPP GEGENWART, and ALEXANDER A. TSIRLIN — Centerfor Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

NaYbO<sub>2</sub> and KYbO<sub>2</sub> feature the same space group  $R\overline{3}m$  as the spinliquid candidate YbMgGaO<sub>4</sub> but evade structural disorder pertinent to that compound. We report a comparative study of these triangular antiferromagnets including their structural characterization and thermodynamic properties in the milli-K temperature range. Both NaYbO<sub>2</sub> and KYbO<sub>2</sub> reveal magnetic interactions of about 4K and no signs of magnetic order in zero field, but undergo field-induced magnetic order that in the Na case occurs between 3T and 8T. By studying specific heat of NaYbO<sub>2</sub> at milli-K temperatures, we conclude that between 0.5T and 2T, within the putative spin-liquid phase, magnetic specific heat follows quadratic behavior expected for the gapless Dirac spin liquid. In zero field, no simple power-law behavior can be observed, but the data clearly deviated from an activated behavior expected for a gapped ground state. Our observations establish gapless nature of the spin-liquid phase of triangular antiferromagnets.

MA 22.3 Tue 10:00 HSZ 304

NMR and bulk magnetometry investigations of the fieldinduced order in the frustrated triangular-lattice compound  $NaYbSe_2 - \bullet S.$  Luther<sup>1,2</sup>, K. M. Ranjith<sup>3</sup>, T. Reimann<sup>1</sup>, Ph. Schlender<sup>4</sup>, B. Schmidt<sup>3</sup>, J. Sichelschmidt<sup>3</sup>, H. Yasuoka<sup>3</sup>, J. Wosnitza<sup>1,2</sup>, Th. Doert<sup>4</sup>, M. Baenitz<sup>3</sup>, and H. Kühne<sup>1</sup> -<sup>1</sup>Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — <sup>2</sup>Institut für Festkörper- und Materialphysik, TU Dresden, Germany — <sup>3</sup>MPI for Chemical Physics of Solids, Dresden, Germany <sup>-4</sup>Faculty of Chemistry and Food Chemistry, TU Dresden, Germany The Yb-based delafossite NaYbSe<sub>2</sub> is a triangular-lattice antiferromagnet with space group (R-3m). In this compound, spin-orbit coupling leads to a pronounced magnetic anisotropy. The absence of magnetic long-range order at zero field is suggestive of 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 revealed, 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 signatures of long-range order down to 0.3 K.

Location: HSZ 304

Spin orbit entangled J = 1/2 triangular magnets NaYbCh<sub>2</sub> (Ch:O,S,Se): pushing a spin liquid into criticality and magnetic order by magnetic fields — •M. BAENITZ<sup>1</sup>, K.M. RANJITH<sup>1</sup>, S. LUTHER<sup>3</sup>, PH. SCHLENDER<sup>2</sup>, T. REIMANN<sup>3</sup>, S. KHIM<sup>1</sup>, J. SICHELSCHMIDT<sup>1</sup>, B. SCHMIDT<sup>1</sup>, H. YASUOKA<sup>1</sup>, H. KUEHNE<sup>3</sup>, J. WOSNITZA<sup>3</sup>, and TH. DOERT<sup>2</sup> — <sup>1</sup>MPI for Chemical Physics of Solids, D-01187 Dresden, Germany — <sup>2</sup>TU Dresden, Department of Chemistry and Food Chemistry, D-01062 Dresden, Germany — <sup>3</sup>Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, D- 01328 Dresden, Germany

Spin orbit coupling (SOC) brought significant progress to the field of quantum spin liquids (QSLs). Yb-based magnets are prime candidates for the QSL-state and as such the NaYbCh<sub>2</sub> series is regarded as a unique platform to study anisotropic planar spin 1/2 triangular lattice magnetism (TLM) with bond frustration. In contrast to YbMgGaO<sub>4</sub>,which shares the same space group (R-3m), NaYbCh<sub>2</sub> lacks inherent lattice distortions and Yb resides on a centrosymmetric position in the YbCh<sub>6</sub> octahedron. Our comprehensive study combines bulk- and local- probes and identifies NaYbCh<sub>2</sub> as a new class of spin orbit entangled TLMs were the QSL state is realized on a perfect triangular lattice [1,2]. The application of fields in (a,b)-plane transforms the system into a critical regime followed by long range order. We present magnetization, specific heat and Na NMR data down to 300 mK

M. Baenitz et al., Phys. Rev. B 98 (2018)
K.M. Ranjith et al., Phys. Rev. B 99 (2019)

MA 22.5 Tue 10:30 HSZ 304 Spin dynamics in the quantum spin liquid candidate Na<sub>2</sub>BaCo(PO<sub>4</sub>)<sub>2</sub> probed by Electron Spin Resonance — •CHRISTOPH WELLM<sup>1,2</sup>, WILLI ROSCHER<sup>1</sup>, VLADISLAV KATAEV<sup>1</sup>, OLEG JANSON<sup>1</sup>, BERND BÜCHNER<sup>1,2</sup>, ROBERT J. CAVA<sup>3</sup>, and RUIDAN ZHONG<sup>3</sup> — <sup>1</sup>Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01069 — <sup>2</sup>Institut für Festkörper- und Materialphysik, Technische Universität Dresden, D-01062 — <sup>3</sup>Department of Chemistry, Princeton University, Princeton, US-08544

The triangular-lattice magnet  $Na_2BaCo(PO_4)_2$  with localized effective spin-1/2 moments of  $Co^{2+}$  ions shows strong, exotic magnetic flucuations in absence of long-range order down to 0.3 K with large residual entropy and linear in temperature spinon excitations, making it a very promising candidate for the realization of a quantum spin liquid [1,2]. We report electron spin resonance (ESR) and magnetization results of powder and single crystals of the title compound supporting the scenario of a spin liquid. We relate our results to previous experimental studies [1,2] and theory (talk by W. Roscher et.al. at this conference). [1] R. Zhong *et al.*, Proc. Natl. Acad. Sci., **116**, pp. 14505-14510 (2019)

[2] N. Li *et al.*, arXiv:1911.11107 (2019)

MA 22.6 Tue 10:45 HSZ 304 DFT calculations of the quantum spin liquid candidate Na<sub>2</sub>BaCo(PO<sub>4</sub>)<sub>2</sub> – •WILLI ROSCHER, CHRISTOPH WELLM, BERND BÜCHNER, VLADISLAV KATAEV, and OLEG JANSON — Leibniz Institute for Solid State and Materials Research Dresden, Germany

The recently synthesized triangular lattice magnet Na<sub>2</sub>BaCo(PO<sub>4</sub>)<sub>2</sub> shows effective S = 1/2 behavior with strong quantum fluctuations persistent down to 50 mK, rendering it as a candidate for the quantum spin liquid (QSL) ground state [1,2]. Very recent ESR and magnetization measurements hint at a more complex picture with different energy scales. To provide a microscopic insight, we perform band structure DFT calculations using the full-potential code FPLO. We calculate the band structure and Wannier projections for the  $t_{2g}$  an  $e_g$ states of Co. The evaluated transfer integrals are used to estimate the leading magnetic exchanges, the spin orbit coupling constant and the trigonal crystal field splitting. These two latter parameters are used to assess the electronic ground state and the excitation spectrum of  $Co^{2+}$  atoms. Finally, we compare our theoretical findings with new experimental studies.

 R. Zhong *et al.*, Proc. Natl. Acad. Sci., **116**, pp. 14505-14510 (2019)

[2] N. Li et al., arXiv:1911.11107 (2019)

MA 22.7 Tue 11:00 HSZ 304 Evidence of one-dimensional magnetic heat transport in the triangular-lattice antiferromagnet  $Cs_2CuCl_4$  – – E. Schulze<sup>1,2</sup>, S. Arsenijevic<sup>1</sup>, L. Opherden<sup>1</sup>, A.N. Ponomaryov<sup>1</sup>, J. Wosnitza<sup>1,2</sup>, T. Ono<sup>3</sup>, H. Tanaka<sup>4</sup>, and  $\bullet$ S.A. Zvyagin<sup>1</sup> – <sup>1</sup>Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, 01328 Dresden, Germany — <sup>2</sup>TU Dresden, 01062 Dresden, Germany <sup>3</sup>Osaka Prefecture University, Osaka 599-8531, Japan — <sup>4</sup>Tokyo Institute of Technology, Tokyo 152-8551, Japan

We report on low-temperature heat-transport properties of the spin-1/2 triangular-lattice antiferromagnet Cs<sub>2</sub>CuCl<sub>4</sub>. Broad maxima in the thermal conductivity along the three principal axes, observed at about 5 K, are interpreted in terms of the Debye model, including the phonon Umklapp scattering. For thermal transport along the b axis, we found a pronounced field-dependent anomaly, close to the transition into the three-dimensional long-range-ordered state. No such anomalies were observed for the transport along the a and c directions. We argue that this anisotropic behavior is related to an additional heattransport channel through magnetic excitations, that can best propagate along the direction of the largest exchange interaction. Our observations strongly support the quasi-1D spin-liquid scenario with spinons as elementary excitations, proposed for this frustrated antiferromagnet. Besides, peculiarities of the heat transport of Cs<sub>2</sub>CuCl<sub>4</sub>in magnetic fields up to the saturation field and above are discussed [1]. This work was supported by the DFG.

[1] E. Schulze et al., Phys. Rev. Research 1, 032022(R) (2019).

## 15 min. break.

MA 22.8 Tue 11:30 HSZ 304 Thermal conductivity of the hyper-hyperkagome spin liquid candidate  $PbCuTe_2O_6$  — •Xiaochen Hong<sup>1</sup>, Matthias GILLIG<sup>1</sup>, SHRAVANI CHILLAL<sup>2</sup>, A. T. M. NAZMUL ISLAM<sup>2</sup>, BERND BÜCHNER<sup>1,3,4</sup>, BELLA LAKE<sup>2,5</sup>, and CHRISTIAN HESS<sup>1,4</sup> - <sup>1</sup>Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden (IFW- Dresden), Dresden — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — <sup>3</sup>Institute of Solid State Physics, TU Dresden, Dresden — <sup>4</sup>Center for Transport and Device, TU Dresden, Dresden – <sup>5</sup>Technische Universität Berlin, Berlin

Quantum spin liquids (QSLs) are exotic phases of matter formed by interacting quantum spins. QSLs are characterized by the absence of static magnetism and the existence of emergent fractional excitations. Recently, PbCuTe<sub>2</sub>O<sub>6</sub> was discovered to be a rare QSL candidate with a three-dimensional spin structure. Here we report the thermal conductivity measurements of this compound down to about 50 mK and up to 16 T. Our results show evidence for the gapped spinons in PbCuTe<sub>2</sub>O<sub>6</sub>. Besides, the unusual field dependence of its low temperature thermal conductivity indicates the residual magnetic order is very sensitive to the external field.

MA 22.9 Tue 11:45 HSZ 304

Probing anisotropic static and dynamic magnetic interactions of Fe-kagome  $Fe_4Si_2Sn_7O_{16}$  by bulk magnetisation and NMR — ●S. DENGRE<sup>1</sup>, R. SARKAR<sup>1</sup>, L. OPHERDEN<sup>2</sup>, M. UHLARZ<sup>2</sup>, T. HERRMANNSDÖRFER<sup>2</sup>, M. ALLISON.<sup>3</sup>, T. SÖHNEL<sup>3</sup>, C.D. LING<sup>4</sup>, J GARDNER<sup>5</sup>, and H.-H. KLAUSS<sup>1</sup> — <sup>1</sup>Institute of Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany — <br/>  $^2 \mathrm{Institute}$ of Resource Ecology and Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Germany <sup>3</sup>School of Chemical Sciences, University of Auckland, Auckland 1142, New Zealand —  $^4$ School of Chemistry, The University of Sydney, Sydney 2006, Australia — <sup>5</sup>Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organization, Menai 2234, Australia

 $Fe_4Si_2Sn_7O_{16}$  hosts an undistorted kagome lattice with  $Fe^{2+}$  (3d<sup>6</sup>, S=2) spins. We present results on oriented and unoriented powder samples. The bulk magnetic susceptibility shows the presence of strong planar (XY) rather than *Ising* anisotropy. Both static NMR shift (K)and dynamic spin-lattice relaxation rate  $(1/T_1)$  NMR reveal a highly anisotropic behaviour in  $\parallel$  and  $\perp$  orientation of the external field with respect to the Kagome planes. For  $\parallel$  orientation, the NMR shift (K) scales linearly with the bulk susceptibility for temperatures ranging from 100 K to 4 K. The NMR shift in  $\perp$  orientation shows the onset of AFM correlations at T  $\approx$  30 K by a deviation from the linear scaling. This is also reflected in the  $1/T_1$  for  $\parallel$  orientation, which starts to decrease at T  $\approx$  30 K.

MA 22.10 Tue 12:00 HSZ 304 Dynamics of an SU(2)-symmetric Kitaev model: spectroscopic signatures of fermionic magnons —  $\bullet$ WILLIAN MASSASHI HISANO NATORI<sup>1</sup> and JOHANNES KNOLLE<sup>1,2,3</sup> — <sup>1</sup>Imperial College London, London, United Kingdom — <sup>2</sup>Technische Universitat Munchen, Garching, Germany — <sup>3</sup>Munich Center for Quantum Science and Technology, Munich, Germany

In this work, we study the dynamics of an integrable Kugel-Khomskii Hamiltonian defined as an extension of the Kitaev honeycomb model. This model displays a global SU(2) symmetry that leads to S=1fermionic excitations. We show that these fermions' dynamical response is exactly computed using a few-particle approach and can be experimentally probed with resonant inelastic x-ray scattering. The techniques developed to uncover the dynamics of the Kitaev model are used to compute the expected neutron scattering response. We show that the SU(2) symmetric model exhibits a vison gap three times larger than the spin-1/2 Kitaev model and a broader band of excitations due to the presence of additional Majorana flavors.

MA 22.11 Tue 12:15 HSZ 304 Phonon renormalization in the Kitaev quantum spin liquid •Alexandros Metavitsiadis and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany

We present the self-energy of phonons, magnetoelastically coupled to the two-dimensional Kitaev spin-model on the honeycomb lattice. Fractionalization of magnetic moments into mobile Majorana matter and a static  $\mathbb{Z}_2$  gauge field lead to a continuum of relaxation processes comprising two channels. Thermal flux excitations, which act as an emergent disorder, strongly affect the phonon renormalization. Above the flux proliferation temperature, the dispersion of a narrow quasiparticle-hole channel is suppressed in favor of broad and only weakly momentum dependent features, covering large spectral ranges. Our analysis is based on complementary calculations in the low-temperature homogeneous gauge and a mean-field treatment of thermal gauge fluctuations, valid at intermediate and high temperatures.

MA 22.12 Tue 12:30 HSZ 304 Phase Diagram of the Breathing Kagome S = 1/2 XY Model with Four-Site Ring Exchange - • NIKLAS CASPER and WOL-FRAM BRENIG — Institute for Theoretical Physics, Technical University Braunschweig, Germany

We study the phase diagram of the breathing kagome S = 1/2 XY model with four-site ring exchange. This model exhibits trimerization of the nearest neighbor exchange between up-/downward oriented triangles of the kagome lattice. This may be of relevance to compounds like vanadium oxyfluoride  $[NH_4]_2[C_7H_{14}N][V_7O_6F_{18}]$ .

Though a frustrated quantum spin model, it does not suffer from the sign problem and therefore can be treated by quantum Monte Carlo. In particular, we use the stochastic series expansion method which is extended to treat four-site ring exchange terms residing on the up to next nearest neighbor bow-tie plaquettes by using an update procedure proposed by Roger G. Melko and Anders W. Sandvik [Phys. Rev. E 72, 026702].

Results for the spin stiffness will be presented in order to study the quantum phase transition belonging to the 3D XY universality class.

MA 22.13 Tue 12:45 HSZ 304

Chromium breathing pyrochlores as a showcase for a variety of pyrochlore Hamiltonians — • TOBIAS MÜLLER<sup>1</sup>, PRATYAY GHOSH<sup>2</sup>, YASIR IQBAL<sup>3</sup>, RONNY THOMALE<sup>1</sup>, JOHANNES REUTHER<sup>4</sup>, MICHEL J. P. GINGRAS<sup>5,6</sup>, and HARALD O. JESCHKE<sup>7</sup> — <sup>1</sup>Institute for Theoretical Physics and Astrophysics, Julius-Maximilians University of Würzburg, Am Hubland, D-97074 Würzburg, Germany -<sup>2</sup>Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen PSI, Schweiz Switzerland — <sup>3</sup>Department of Physics, Indian Institute of Technology Madras, Chennai 600036, India — <sup>4</sup>Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germa — <sup>5</sup>epartment of Physics and Astronomy, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada  $^{6}\mathrm{Quantum}$  Materials Program, Canadian Institute for Advanced Research, MaRS Centre, West Tower 661 University Ave., Suite 505, Toronto, ON, M5G 1M1, Cana — <sup>7</sup>Research Institute for Interdisciplinary Science, Okayama University, Okayama 700-8530, Japa

We investigate all six structurally characterized chromium-based

breathing pyrochlores using a combination of density functional theory and pseudofermion functional renormalization group calculations. We show that the variety of chemical compositions leads to distinct magnetic behavior due to the different pyrochlore Hamiltonians realized. We discuss especially the line-like degeneracies in momentum space found in sulfide compounds and an approximate spiral spin liquid in a selenide material. The root cause for these effects are longer-rage exchange couplings up to third nearest neighbor type.