# TT 17: Correlated Electrons: Spin Systems, Itinerant Magnets 2

Time: Monday 15:00–17:45 Location: H19

TT 17.1 Mon 15:00 H19

**Entanglement Entropy and Quantum Monte Carlo** — •Peter Bröcker — Institut für Theoretische Physik, Universität zu Köln

Entanglement spectra and entanglement entropies have attracted a lot of attention in the last few years. Among other things, they can serve as precise indicators for (quantum) phase transitions as well as for detecting topologically ordered phases. We will report on the calculation of entanglement entropies in Quantum Monte Carlo, in particular in the frameworks of Loop Quantum Monte Carlo and Stochastic Series Expansion. We will also discuss approaches for Auxiliary Field Quantum Monte Carlo, which is of special interest in light of recent advances in simulations of fermionic models in the vicinity of the antiferromagnetic phase transition.

TT 17.2 Mon 15:15 H19

**The phase diagram of the two-orbital Hubbard model by means of the dynamical mean field theory** — •Vlastimil Křápek and Jan Kuneš — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, 162 00 Praha, Czech Republic

The Blume-Emery-Griffiths (BEG) model with repulsive biquadratic coupling exhibits a complex multicritical phase diagram [1]. In our recent work we have shown that the two-orbital Hubbard model can be mapped on BEG model when only certain nearest-neighbor interactions are considered and that this model is relevant for the spin-state transition observed in LaCoO3 [2].

Motivated by this we explore the phase diagram of the two-orbital Hubbard model further, focusing on the following points: (1) By changing the bandwidths we can vary the metallicity of the system while keeping the parameters of the BEG model constant. (2) By changing the temperature and the crystal-field splitting we visit different phases and study the transitions between them. The two-site unit cell is used to allow for the orbital and magnetic ordering. (3) We study the effect of the number of electrons different from the half filling.

[1] W. Hoston and A. N. Berker, Phys. Rev. Lett. 67, 1027 (1991).
[2] J. Kuneš and V. Křápek, Phys. Rev. Lett. 106, 256401 (2011).

TT 17.3 Mon 15:30 H19

**Towards microscopic understanding of skyrmions in $Cu_2OSeO_3$: an effective theory description** — Oleg Janson[1], •Ioannis Rousochatzakis[2], Alexander Tsirlin[3], Ulrich Rössler[2], Jeroen van den Brink[2], and Helge Rosner[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [3]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

We present a quantitative physical picture for the spin 1/2 ferrimagnetic helimagnet $Cu_2OSeO_3$ based on a DFT-based microscopic magnetic model. Besides clarifying the relevant low-energy magnetic degrees of freedom, the main successes of the theory are the following: (i) it reveals an intimate connection between $Cu_2OSeO_3$ (an insulating ferrimagnet) and MnSi (a metallic ferromagnet); (ii) it clarifies which Dzyaloshinskii-Moriya terms are responsible for the long-wavelength twisting, and gives a helix period of 58 nm, in very good agreement to the one ($\sim$50 nm) reported by Lorentz transmission electron microscopy by Seki *et al* [1]; (iii) it predicts the presence of a small antiferromagnetic canting which is tied to the long-wavelength twisting; (iv) it reveals the mechanism for the reduction of the Cu moments as observed by Bos *et al* [2].

[1] S. Seki, X. Z. Yu, S. Ishiwata, Y. Tokura, Science **336**, 198 (2012)
[2] J.-W. G. Bos, C. Colin, T. Palstra, Phys. Rev. B **78**, 094416 (2008).

TT 17.4 Mon 15:45 H19

**Towards microscopic understanding of skyrmions in $Cu_2OSeO_3$: a DFT study** — •Oleg Janson[1], Ioannis Rousochatzakis[2], Alexander Tsirlin[1,3], Ulrich Rössler[2], Jeroen van den Brink[2], and Helge Rosner[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [3]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

Unlike most undoped cuprates, the $S = 1/2$ Heisenberg magnet $Cu_2OSeO_3$ exhibits a ferrimagnetic ground state and a sizable magnetoelectric coupling. Furthermore, recent experimental studies reported magnetic-field-induced emergence of skyrmions in this insulating material. Based on extensive DFT band structure calculations, we evaluate the microscopic magnetic model, including isotropic (Heisenberg) and anisotropic (Dzyaloshinskii-Moriya) terms. We extract five relevant magnetic couplings that form a complex, but non-frustrated spin model which can be described as a pyrochlore lattice of magnetic tetrahedra. The model parameters are justified by quantum Monte-Carlo simulations and subsequent comparison to the experiments.

TT 17.5 Mon 16:00 H19

**Long-wavelength helimanegtic order and skyrmion lattice phase in $Cu_2OSeO_3$** — Alfonso Chacon[1,2], •Tim Adams[1], Michael Wagner[1], Andreas Bauer[1], Georg Brandl[1,2], Bjoern Pedersen[2], Helmuth Berger[3], Peter Lemmens[4], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik-Department E21, D-85748 Garching, Germany — [2]Forschungsneutronenquelle Heinz Maier Leibnitz (FRM II), Lichtenbergstr. 1, 85748 Garching, Germany — [3]Ecole Polytechnique Federale Lausanne, CH-1015 Lausanne, Switzerland — [4]Institute for Condensed Matter Physics, TU Braunschweig, D-38106 Braunschweig, Germany

We report a long-wavelength helimagnetic superstructure in bulk samples of the ferrimagnetic insulator $Cu_2OSeO_3$. The magnetic phase diagram associated with the helimagnetic modulation inferred from small-angle neutron scattering and magnetization measurements includes a skyrmion lattice phase and is strongly reminiscent of MnSi, FeGe, and $Fe_{1-x}Co_xSi$, i.e., binary isostructural siblings of $Cu_2OSeO_3$ that order helimagnetically. The temperature dependence of the specific heat of $Cu_2OSeO_3$ is characteristic of nearly critical spin fluctuations at the helimagnetic transition. This provides putative evidence for effective spin currents as the origin of enhancements of the magnetodielectric response instead of atomic displacements considered so far.

TT 17.6 Mon 16:15 H19

**Mössbauer, NMR und $\mu$SR investigations of microscopic magnetic ordering of $La_2O_2Fe_2OSe_2$** — •Sirko Bubel[1], Marco Günther[1], Rajib Sarkar[1], Hans-Henning Klauss[1], Hubertus Luetkens[2], Gwendolyn Pascua[2], Kwang-Yong Choi[3], and Haidong Zhou[4] — [1]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [3]Institut für Physik der Kondensierten Materie, 38106 Braunschweig, Germany — [4]Experimental Condensed Matter Physics, University of Tennesee

20 years after the first investigations of the antiferromagnetically ordered oxo-chalcogenid $La_2O_2Fe_2OSe_2$ the common picture of microscopic alignment of iron moments in the expanded squarish $Fe_2O$-layers is still controversy discussed [1,2]. Furthermore first superconducting samples of this structural class were succesully synthesized in 2012 [3] linking this oxo-chalcogenid to the pnictide superconductors.

To understand the mechanism of iron magnetism in these systems we investigated a powder sample of $La_2O_2Fe_2OSe_2$ by $^{57}$Fe-Mössbauer spectroscopy, $\mu$SR and $^{139}$La-NMR. These measurements strongly suggest that iron moments are coupled ferromagnetically via selenium and antiferromagnetically via oxygen. We infer a new magnetic structure on the basis of these results, being consistent with Goodenough-Kanamori-rules, and speculate about orbital order in this system.

[1] Y. Fuwa *et al.*, Phys. Rev. B. **84** (2011) 174506
[2] D. J. Free, S. O. Evans, Phys. Rev. B. **81** (2010) 214433
[3] P. Doan *et al.*, J. Am. Chem. Soc. **134**, 16520 (2012)

**15 min. break**

**Topical Talk** TT 17.7 Mon 16:45 H19

**Magnetic Frustration in a Quantum Spin Chain: The Case of Linarite $PbCuSO_4(OH)_2$** — •Anja U.B. Wolter[1], Markus Schäpers[1], Ferdinand Lipps[1], Vladik Kataev[1], Satoshi Nishimoto[1], Stefan-Ludwig Drechsler[1], Bernd Büchner[1], Rico Beyer[2], Marc Uhlarz[2], Jochen Wosnitza[2], Britta

Willenberg[3], Manfred Reehuis[3], Kirrily C. Rule[3], Bachir Ouladdiaf[4], and Stefan Süllow[5] — [1]Leibniz-Institut IFW Dresden, Dresden, Germany — [2]Dresden High Magnetic Field Laboratory, Dresden, Germany — [3]Dresden High Magnetic Field Laboratory, Dresden, Germany — [4]Institute Laue-Langevin, Grenoble, France — [5]IPKM, TU Braunschweig, Braunschweig, Germany

We present a combined neutron diffraction, NMR and bulk thermodynamic study of the natural mineral linarite $PbCuSO_4(OH)_2$. An incommensurate magnetic ordering with a propagation vector k=(0,0.186,1/2) was found below $T_N$=2.8 K in a zero magnetic field. The analysis of the neutron diffraction data yields an elliptical helical structure. From detailed investigations of linarite in magnetic fields up to 12 T, applied along the chain direction, a very rich magnetic phase diagram is established, with multiple field-induced phases, and possibly short-range-order effects occurring in high fields. Our data establish linarite as a model compound of the frustrated one-dimensional spin chain, with ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor interactions. Long-range magnetic order is brought about by interchain coupling one order of magnitude smaller than the intrachain coupling.

TT 17.8 Mon 17:15 H19

**Investigation of Ferromagnetic Copper Oxides** — •Kevin Caslin[1], Reinhard Kremer[1], Mike Whangbo[2], Jia Liu[2], and Franz Pertlik[3] — [1]MPI für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Dept. of Chemistry, North Carolina State Univ., Raleigh, North Carolina 27695-8204, USA — [3]Inst. f. Mineralogie und Kristallographie d. Univ., A-1010 Wien, Österreich

We are investigating low dimensional $S = \frac{1}{2}$ Cu quantum-chain systems. Materials containing Cu $S = \frac{1}{2}$ moments in a distorted oxygen octahedral environment form $CuO_2$ ribbon chains. Such ribbon chains support ferromagnetic (FM) nearest-neighbour (NN) via Cu-O-Cu exchange and antiferromagnetic (AFM) next-nearest-neighbour (NNN) via Cu-O-O-Cu exchange. Often the NNN-AFM interaction is dominant and leads to a low temperature, AFM, long-range ordering. Systems of this type are known to develop unusual structural distortions and incommensurate spiral magnetic structures.[1,2,3] In this study, we search for $S = \frac{1}{2}$ Cu based materials with crystal structures leading to a predominate NN-FM exchange. X-ray diffraction, heat capacity, thermal expansion and magnetic measurements were performed to characterize such materials. DFT and band structure calculations were also carried out for further invesitgation.

[1] B. J. Gibson, R. K. Kremer, A. V. Prokofiev, W. Assmus, and G. J. McIntyre, Physica B **350**, E253 (2004)
[2] C. Lee, Jia Liu, M.-H Whangbo, H.-J. Koo, R. K. Kremer, and A. Simon, Phys. Rev. B **86**, 060407 (2012)
[3] M. G. Banks, R. K. Kremer, C. Hoch, A. Simon, B. Ouladdiaf, J.-M. Broto, H. Rakoto, C. Lee, and M.-H. Whangbo, Phys. Rev. B **80**, 024404 (2009)

TT 17.9 Mon 17:30 H19

**Quantum helimagnets: detriments and new chances for multipolar phases** — Satoshi Nishimoto[1], •Stefan-Ludwig Drechsler[1], Roman Kuzian[2], Johannes Richter[3], and Jeroen van den Brink[1] — [1]Institut für Theoretische Festkörperphysik am IFW-Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Institute for Materials Science, Kiiv, Ukraine — [3]Universiät Magdeburg, Institut für Theoretische Physik, Germany

Arbitrarily strong coupled frustrated spin-1/2 chains in high magnetic fields described within the ferro- antiferromagnetic $J_1$-$J_2$ Heisenberg model and various types of interchain coupling are studied by DMRG, hard-core boson, and spin-wave theory approaches. Multipolar phases related to multimagnon bound states are destroyed (supported) by weak antiferromagnetic (ferromagnetic) interchain couplings $J_{\rm ic}$. We show that quantum spin nematics (quadrupolar phase) might be found for $LiVCuO_4$ whereas for $Li(Na)Cu_2O_2$ it is prevented by a sizeable antiferromagnetic $J_{\rm ic}$. Instead $PbCuSO_4(OH)_2$ (linarite) with sizable easy-axis anisotropy for ferromagnetic nearest neighbor inchain coupling $J_1$ of about 12% might be a good candidate for a triatic (octupolar) phase.