TT 47: Correlated Electrons: Spin Systems and Itinerant Magnets - Frustrated Magnets III

Time: Tuesday 14:00–16:00 Location: HSZ 03

TT 47.1 Tue 14:00 HSZ 03

Spin Heat-Conductivity of Two-Dimensional Antiferromagnets coupled to Phonons — •Wolfram Brenig[1,2] and Alexander L Chernyshev[3] — [1]Institute for Theoretical Physics, Technical University Braunschweig, Germany — [2]Technical University of Lower Saxony, NTH, Germany — [3]Department of Physics, University of California, Irvine, USA

We present results of a study of thermal transport due to magnons in two dimensional spin-1/2 Heisenberg antiferromagnets on the square lattice, subject to dissipation by lattice degrees of freedom. The spin phonon scattering is described in terms of magnetoelastic coupling to either acoustic of optical lattice modes. The thermal conductivity and transport relaxation rates will be evaluated using both, a memory function approach and Boltzmann equations. The temperature dependence of the transport will be analyzed in terms of various asymptotic scattering processes. Implications for recent observations of magnetic thermal transport in layered cuprate materials will be discussed.

TT 47.2 Tue 14:15 HSZ 03

Spin-current autocorrelations from single pure-state propagation — •Robin Steinigeweg[1], Jochen Gemmer[2], and Wolfram Brenig[1] — [1]Institute for Theoretical Physics, Technical University Braunschweig, Germany — [2]Department of Physics, University of Osnabrück, Germany

We study spin dynamics in the anisotropic and antiferromagnetic spin-1/2 Heisenberg chain in the long-wavelength limit. To this end, we numerically calculate the spin-current autocorrelation function by propagating only a single pure state in time, which is a "typical" representative of the quantum statistical ensemble. By comparing to short-time data from time-dependent density matrix renormalization group, we show that quantum typicality is fulfilled extremely well. This quantum typicality allows us to determine almost exactly the long-time Drude weight for chains as long as $L = 33$ sites, i.e., with a $8192\times$ larger Hilbert space than the typically considered $L \sim 20$ sites within the range of exact diagonalization. Therefore we can shed light on the Drude weight in the thermodynamic limit at both, high and low temperatures. Even though we apply our approach to an integrable quantum system in one dimension, it is applicable to non-integrable models in a much more general framework.

TT 47.3 Tue 14:30 HSZ 03

Microscopic magnetic modeling for the spin-$\frac{1}{2}$ kagome compound $[\mathbf{NH_4}]_2[\mathbf{C_7H_{14}N}][\mathbf{V_7O_6F_{18}}]$ — •Oleg Janson[1,2], Alexander Tsirlin[1,2], Ioannis Rousochatzakis[3], Helge Rosner[1], and Raivo Stern[2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia — [3]Leibniz Institute for Solid State and Materials Research, Dresden, Germany

In the recently synthesised compound $[NH_4]_2[C_7H_{14}N][V_7O_6F_{18}]$, magnetic $S=\frac{1}{2}$ V^{4+} atoms form an ideal kagome lattice [1]. Very recent μSR studies indicate the emergence of a gapless spin liquid state as a result of magnetic frustration [2]. Using density functional theory calculations, we address the microscopic magnetic model of this low-dimensional compound. We show that its peculiar symmetry gives rise to two inequivalent nearest-neighbor couplings. The behavior of the resulting quantum spin model is studied using exact diagonalization and compared to the experiments. OJ and AT were supported by the Mobilitas program of the ESF, grant numbers MJD447 and MTT77, respectively.

[1] F. H. Aidoudi *et al.*, Nature Chem. **3**, 810 (2011)
[2] L. Clark *et al.*, Phys. Rev. Lett. **110**, 207208 (2013)

TT 47.4 Tue 14:45 HSZ 03

The Spin-1 Kagome Antiferromagnet $\mathbf{Ca_{10}(Cr^{V}O_4)_6(Cr^{VI}O_4)}$ — •Christian Balz[1,2], Bella Lake[1,2], Nazmul Islam[1], Manfred Reehuis[1], and Yogesh Singh[3] — [1]Helmholtz Zentrum Berlin, 14109 Berlin, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [3]Indian Institute of Science Education & Research Mohali, 140306 Mohali, India

The mixed valence compound $Ca_{10}(Cr^{V}O_4)_6(Cr^{VI}O_4)$ consists of ferromagnetically coupled pairs of spin-1/2 Cr^{5+} ions which form dimers along the *c*-axis. These dimers form an effective spin-1 Kagome arrangement in the *a*-*b*-plane. Besides Cr^{5+} there are also Cr^{6+} ions in the structure which are non-magnetic. We have grown single crystals of $Ca_{10}(Cr^{V}O_4)_6(Cr^{VI}O_4)$ and have performed DC susceptibility, magnetization and heat capacity measurements as well as powder and single crystal neutron diffraction and powder X-ray diffraction experiments. Our magnetization and diffraction confirm the ordered arrangement of Cr^{5+} and Cr^{6+} ions in the ratio 6:1, while the heat capacity and susceptibility show the absence of long-range magnetic order down to 50 mK. We have also performed inelastic neutron scattering which reveals diffuse excitations which are gapless everywhere and are highly two-dimensional. Two bands of scattering are observed, the low energy band (0-0.7 meV) corresponds to excitations of the spin-1 Kagome and the higher energy band (0.7-1.4 meV) corresponds to excitations of the dimer bond. Thus, the Kagome antiferromagnet $Ca_{10}(Cr^{V}O_4)_6(Cr^{VI}O_4)$ is a promising candidate for a Spin-Liquid ground state.

TT 47.5 Tue 15:00 HSZ 03

Impact of vacancies on the Kagome Antiferromagnet — •Siegfried Guertler — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

The Kagome lattice Heisenberg model, has been the subject of discussions over a long time. Recently strong indication for a spin-liquid ground state has been found numerically. The exact type of spin-liquid is still debated, as is the question whether it is gapped or not.
An interesting point is how perturbations in the form of vacancies change the picture. This is relevant for experimental detection techniques on compounds (photo-doping), the possible design of new compounds (chemical doping) and as well for experiments applying pressure and therefore changing the coupling constants.
In this talk I present numerical investigations by variational Monte-Carlo of the role of vacancies regarding this problem, particularly the t-J and Hubbard model on this lattice. For the t-J model a particular form of a valence bond crystal appears and can be understood by a few observed short range effects (as reported in PRB 84, 174409 (2011) and PRL 111, 097204 (2013)) the Hubbard model in the low-U limit seems to have a rich phase-diagram including various exotic phases and magnetically ordered phases (to appear soon on cond-mat).

TT 47.6 Tue 15:15 HSZ 03

Strongly Correlated Fermions on the Kagome Lattice — •Krishanu Roychowdhury and Frank Pollmann — MPIPKS, Dresden, germany

We consider an extended fermionic Hubbard model on the kagome lattice and show that this model exhibits exciting phenomena at certain fractional filling factors. The strong coupling regime of the model, described by an effective low-energy Hamiltonian, includes competing interactions, i.e., fermionic ring exchange as well as an antiferromagnetic Heisenberg term. We find that the interplay between spin and charge degrees of freedom enforces a quantum phase transition between phases with different spin and charge ordering at 1/3 filling. Following a similar spirit, we also discuss the spin polarized case at 1/6, 1/3 and 1/2 filling and focus on the influence of longer ranged interactions. The possibilities to stabilize topologically ordered phases are explored in detail.

TT 47.7 Tue 15:30 HSZ 03

Investigation of the strongly correlated one-dimensional magnetic behavior of $\mathbf{NiTa_2O_6}$ — •Joseph M Law[1] and Reinhard K Kremer[2] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [2]Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

$NiTa_2O_6$ has been previously shown to be a 2D system.[1] Herein, we re-investigated magnetic properties of $NiTa_2O_6$ by magnetic susceptibility, specific heat, electron paramagnetic resonance, neutron powder diffraction and pulse field magnetization measurements. In contrast to the previous findings we found $NiTa_2O_6$ to be a quasi-1D Heisenberg S = 1 spin chain with a nearest neighbor spin exchange interaction of 18.92(2) K with a g-factor of 2.14(1).
[1] E. G. Santos, J. B. M. da Cunha, O. Isnard, C. Lacroix, and M. A. Gusmao, J. Phys.: Condens. Matter 24, 496004 (2012)

TT 47.8 Tue 15:45 HSZ 03

Flat-band ferromagnetism and Pauli-correlated percolation — •Mykola Maksymenko[1], Andreas Honecker[2], Roderich Moessner[1], Johannes Richter[3], Oleg Derzhko[4], and Kirill Shtengel[5] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen — [3]Institut für theoretische Physik, Universität Magdeburg — [4]Institute for Condensed Matter Physics of NAS of Ukraine — [5]University of California at Riverside

Flat-band ferromagnetism is a special case of magnetism due to correlated itinerant electrons in a number of geometrically frustrated lattices. We develop an exact mapping between ground states of this many-body problem and a novel site-percolation problem. This allows us to study the ferromagnetic transition using tools from equilibrium statistical physics. In the case of the Hubbard model on the Tasaki lattice, we provide a complete analytical treatment of the 1D case and show that for $D > 1$, the paramagnetic phase persists beyond the usual threshhold for uncorrelated percolation point. When the transition to an unsaturated ferromagnetic phase finally occurs, it is in the form of a first-order jump to an unsaturated ferromagnetic phase.