TT 23: Low-Dimensional Systems: Other Materials

Time: Monday 16:45–18:30 Location: BEY 81

TT 23.1 Mon 16:45 BEY 81

Huge magneto-elastic coupling and negative Poisson ratio in low-dimensional spin systems — •Bernd Wolf, Pham Thanh Cong, Rudra Sekhar Manna, Ulrich Tutsch, and Michael Lang — Physikalisches Institut, J.W. Goethe-Universität, SFB/TR49, D-60438 Frankfurt (Main), Germany

Azurite $Cu_3(CO_3)_2(OH)_2$, a model system for the distorted diamond-chain, exhibits pronounced elastic anomalies in the temperature - and magnetic field dependence of the longitudinal elastic mode c_{22}. These features are assigned to the relevant magnetic interactions in the material and their couplings to the lattice degrees of freedom. From a quantitative analysis of the magnetic contribution to c_{22}, the magneto-elastic coupling $G = \partial J_2/\partial\epsilon_b$ is determined, with ϵ_b denoting the strain along the chain b-axis. We find an exceptionally large value highlighting an extraordinarily strong sensitivity of J_2 against changes of the b-axis lattice parameter. These results are complemented by measurements of the hydrostatic pressure dependence of J_2 by means of thermal expansion and magnetic susceptibility measurements performed both at ambient and finite hydrostatic pressure. We discuss the results in light of an anomalous negative Poisson effect at low temperatures. We compare the results with the magneto-elastic coupling constants determined for other low-D quantum spin systems, such as the antiferromagnetic S = 1/2 Heisenberg spin chain based on a Cu-coordination polymer [1], the dimerized spin chain and $SrCu_2(BO_3)_2$ as a coupled quasi-2D system [2].

[1] B. Wolf, et al., Phys. Rev. B **69**, 092403 (2004)
[2] S. Zherlitsyn, et al., Phys. Rev. B **62**, R6097 (2000)

TT 23.2 Mon 17:00 BEY 81

Nuclear Magnetic Resonance on S=1/2 Heisenberg Spin Chains under the Impact of Different Impurities — •Yannic Utz[1], Franziska Hammerath[1], Hans-Joachim Grafe[1], Ashwin Mohan[1], Neela Sekhar Beesetty[2], Romuald Saint-Martin[2], Alexandre Revcolevschi[2], Christian Hess[1], and Bernd Büchner[1] — [1]IFW Dresden, Germany — [2]ILPCES - ICMMO, Université Paris-Sud, France

We present ^{63}Cu NMR measurements on single crystals of undoped, Ni doped and Zn doped $SrCuO_2$ and of Ni doped Sr_2CuO_3. While $SrCuO_2$ forms a double chain structure, the copper ions of Sr_2CuO_3 are arranged as single chains. Despite these structural differences, both are known to be good realizations of the antiferromagnetic S=1/2 Heisenberg chain. The measurements show that Ni doping (S=1) has a major impact on the magnetic properties of both spin chain systems. An unusual line broadening in the low temperature NMR spectra reveals the existence of an impurity-induced local alternating magnetization (LAM), and exponentially decaying spin-lattice relaxation rates T_1^{-1} towards low temperatures indicate the opening of a spin gap similar to Ca-doped $SrCuO_2$ [1]. Zn doping (S=0), however, shows a similar impact on the NMR spectra, but the opening of a spin gap could not be observed. While the different impact of Ni and Zn doping on the spin chains could be explained by their different impurity spins, the opening of a spin gap in case of Ni doping is totally unexpected and not yet understood.

[1] F. Hammerath et al., Phys. Rev. Lett. 107, 017203 (2011)

TT 23.3 Mon 17:15 BEY 81

Hydrogen positions and their effect on exchange couplings of Cu-minerals — •Stefan Lebernegg[1], Alexander Tsirlin[2], Oleg Janson[1,2], and Helge Rosner[1] — [1]MPI Chemical Physics of Solids, Dresden — [2]National Institute of Chemical Physics and Biophysics, Tallinn

Exotic magnetic properties and the possibility of challenging our understanding of collective quantum phenomena are the reasons why low-dimensional spin-1/2 quantum magnets attract so much attention. Cu(2+) minerals belong to this class of compounds where several hundredths of them are provided by nature. However, only very few of them have ever been investigated with respect to their magnetic properties. Thus, the Cu-minerals keep a high potential for the discovery of new effects and materials. However, many of these compounds contain crystal water or OH groups where the position of hydrogen in the crystal structure crucially affects the magnetic behavior. Since the experimental determination of H-positions is highly elaborating if possible at all, these positions are usually not available in the structural data of minerals. We will, thus, present a valuable DFT-based alternative for determining the hydrogen positions. Then, the importance of the hydrogen positions for the magnetic properties and the computation of microscopic magnetic models will be discussed for selected Cu-minerals which have been investigated by combining several experimental and computational techniques.

TT 23.4 Mon 17:30 BEY 81

Magnetic excitation spectra of the 4-leg ladder $La_2Cu_2O_5$ — •Ignacio Vergara[1], Kris Cöster[2], Luis Fels[1], Martin Valldor[1,3], Stefan Wessel[4], Kai Philip Schimdt[2], and Markus Grüninger[1] — [1]II. Physicalisches Institut, Universität zu Köln — [2]Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund — [3]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Institut für Theoretische Festkörperphysik, JARA-FIT and JARA-HPC, RWTH Aachen University

In low-dimensional spin-1/2 cuprates, optical spectroscopy has been established as a powerful tool for the study of magnetic excitations with total S=0. The simultaneous excitation of a symmetry-breaking phonon allows us to study the magnetic excitations at high energies ($\sim$ 0.1 - 1 eV) throughout the entire Brillouin zone, since the phonon ensures momentum conservation. The line shape of the optical conductivity provides important information on the kinetics and on the interactions of the magnetic excitations.

The magnetism of n-leg S=1/2 cuprate ladders is particularly interesting due to the dimensional crossover between 1D and 2D and the possible relevance for high T_c superconductivity. We present optical conductivity data of the 4-leg ladder $La_2Cu_2O_5$ for polarization of the electric field parallel to the legs and to the rungs, respectively. Comparison with theory (CUT, QMC) and with the results for a 2-leg ladder suggests the existence of two-triplon bound states below the continuum also for n=4.

TT 23.5 Mon 17:45 BEY 81

Electronic instabilities of the AA-honeycomb bilayer — •David Sanchez de la Peña[1], Michael M Scherer[2], and Carsten Honerkamp[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]Institute for Theoretical Physics, Heidelberg University, Germany

We use a functional renormalization group approach to study the instabilities due to electron-electron interactions in a bilayer honeycomb lattice model with AA stacking, as it might be relevant for layered graphene. Starting with a tight-binding description for the four π-bands, we integrate out the modes of the dispersion by successively lowering an infrared cutoff and determine the leading tendencies in the effective interactions. The antiferromagnetic spin-density wave is an expected instability for dominant local repulsions among the electrons, but for nonlocal interaction terms also other instabilities occur. We discuss the phase diagrams depending on the model parameters. We compare our results to single-layer graphene and the more common AB-stacked bilayer, both qualitatively and quantitatively.

TT 23.6 Mon 18:00 BEY 81

Susceptibility measurements on a weakly coupled spin-dimer system consisting of nitronyl-nitroxid stable biradicals — •L. Postulka[1], B. Wolf[1], U. Tutsch[1], P.T. Cong[1], M. Baumgarten[2], Y. Borozdina[2], D. Strassel[3], S. Eggert[3], and M. Lang[1] — [1]Physics Institute, Uni Frankfurt SFB/TR 49, D-60438 Frankfurt, Germany — [2]MPI for Polymer Research SFB/TR 49, D-55128 Mainz, Germany — [3]Physics Department and Research Center OPTIMA SFB/TR 49, Uni Kaiserslautern, D-67663 Kaiserslautern, Germany

We present low-temperature susceptibility data on a spin $S = \frac{1}{2}$ dimer system consisting of nitronyl-nitroxid radicals which are bridged via tolan molecules. The material, exhibiting a double-layer structure, can be regarded as a quasi- 2D system. From SQUID magnetisation measurements on high-quality single crystals, an intra-dimer coupling constant of $J_{intra}/k_B \approx 9.6\,\mathrm{K}$ can be determined. In addition, the data reveal indications for an inter-dimer coupling of the order of 1 K. In order to look for magnetic field-induced ordering phenomena, AC-susceptibility measurements were performed down to temperatures as low as $T = 34\,\mathrm{mK}$ and magnetic fields up to $B = 10.5\,\mathrm{T}$. For tem-

peratures below $T = 250\,\mathrm{mK}$, a double-peak structure was observed at fields between 8 T and 9.5 T consistent with the expectation based on the above-mentioned coupling constants. Furthermore, in the same temperature range another anomaly around $B = 4.5\,\mathrm{T}$ appears. For a detailed understanding especially with regard to the dimensionality of the interactions and the implications for the type of order that is realized here, Quantum Monte Carlo simulations are underway.

TT 23.7 Mon 18:15 BEY 81

Orbital contribution to spin-Peierls transition in $TiPO_4$ — Dirk Wulferding[1], Angela Moeller[2], Kwang-Yong Choi[3], Yurii Pashkevich[4], Roman Babkin[4], Karina Lamonova[4], •Peter Lemmens[1], Joseph Law[5], Reinhardt Kremer[6], and Robert Glaum[7] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]Dept. Chem., Univ., Houston, USA — [3]Dept. Phys., CA Univ., Seoul, Korea — [4]DonFTI, Donetsk, Ukraine — [5]Dresden HMFL, Dresden, Germany — [6]MPI-FKF, Stuttgart, Germany — [7]IAC, Bonn, Germany

We observe unusual lattice dynamics as well as evidence for an orbital instability preceding the spin-Peierls transition in $TiPO_4$. Furthermore, there exist high energy excitations of mixed electronic and lattice origin that suggest an exotic dimerization process, different from other spin-Peierls materials. Therefore, the energy gain is related to magnetoelastic and orbital contributions.