TT 32 Correlated Electrons - Low-dimensional Materials II

Zeit: Dienstag 16:15–18:30 Raum: TU H2053

TT 32.1 Di 16:15 TU H2053

Magnetic ground state of the quantum spin magnet $CaCu_2O_3$ probed by high field ESR — •V. Kataev[1], M. Goiran[2], M. Costes[2], J. M. Broto[2], F. C. Chou[3], E. Arushanov[1,2], S. Drechsler[1], and B. Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany — [2]Laboratoire National des Champs Magnétiques Pulsés, 31432 Toulouse Cedex 04, France — [3]Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139, USA

We report an electron spin resonance (ESR) study of the $S = 1/2$-Heisenberg pseudo-ladder magnet $CaCu_2O_3$ in pulsed magnetic fields up to 40 T. At sub-Terahertz frequencies we observe an ESR signal originating from a small amount of uncompensated spins residing presumably at the imperfections of the strongly antiferromagnetically correlated host spin lattice. The data give evidence that these few percent of extra spin states are coupled strongly to the bulk spins and are involved in the antiferromagnetic ordering at $T_N = 25$ K. By mapping the frequency/resonance field diagram we have determined the spin gap for magnetic excitations below T_N amounting to $\sim$0.3 meV. The small value of the gap explains the occurrence of the spin-flop transition in $CaCu_2O_3$ at the critical magnetic field $H_{sp} \sim 3$ T. Qualitative changes of the ESR response with increasing the field strength give indications that strong magnetic fields reduce antiferromagnetic fluctuations and may even suppress the long-range magnetic order in $CaCu_2O_3$. ESR data support theoretical predictions of a significant role of the extra spin states for the properties of the low-dimensional quantum magnets.

TT 32.2 Di 16:30 TU H2053

Evidence for "ferromagnetic" helimagnetism in compounds with frustrated edge-shared CuO_2 chains — •S.-L. Drechsler[1], J. Richter[2], J. Málek[1], A. Moskvin[3], H. Rosner[4], A. Gippius[5], R.E. Kremer[6], and M. Enderle[7] — [1]IFW-Dresden — [2]Universität Magdeburg — [3]Ural State University Ekaterinburg, Russia — [4]MPI f. CPfS, Dresden — [5]State University, Moscow, Russia — [6]MPI f. Festkörperforsch., Stuttgart — [7]Inst. Laue-Langevin, Grenoble, France

We present a combined theoretical and experimental study of the electronic structure and helimagnetism in compounds with frustrated edge-shared CuO_2 chains: $LiVCuO_4$ and $LiCu_2O_2$ vs. the ferromagnetic (fm) inchain ordering in Li_2CuO_2. Based on full potential L(S)DA and LSDA+U band structure calculations, exact diagonalization studies of multi-band Hubbard and Heisenberg models, we estimate sign and magnitude of the most relevant exchange integrals J. Strongly competing fm nearest neighbor (nn) and anti-fm next nn J's are found for the inchain direction. This frustration scenario well describes magnetic susceptibility, specific heat, spin entropy, inelastic neutron scattering, and NMR data. The influence of interchain couplings is briefly discussed.

TT 32.3 Di 16:45 TU H2053

One-dimensional magnetic thermal conductivity of Ca-doped $SrCuO_2$ — •Patrick Ribeiro[1], Christian Hess[2], and Bernd Büchner[1] — [1]IFW-Dresden, Germany — [2]DPMC-Geneva, Switzerland

We present results on the heat conduction of the Ca-doped $SrCuO_2$-system, which is a prototype system for spin 1/2 Heisenberg-chains. 1D-magnetic heat transport is present in this compound, giving rise to a strong anisotropy of the heat conduction tensor. The separation of the magnetic contributions from the phonon background is ambiguous in the pure material $SrCuO_2$. By doping it with Ca, the phononic contribution to the heat conduction is partially suppressed by enhanced phonon-defect scattering. Concomitantly, the electronic configuration of Cu is only weakly affected, since Ca is isovalent to Sr. Hence, no strong changes in the magnetic conductivity are to be expected. This leads to a better separation of both contributions. First results of the thereby obtained magnetic heat conduction will be presented and discussed.

TT 32.4 Di 17:00 TU H2053

Thermal conductivity of single-layered cuprates R_2CuO_4 — •K. Berggold[1], T. Lorenz[1], M. Hofmann[1], J. Baier[1], M. Kriener[1], H. Roth[1], A. Freimuth[1], and S. Barilo[2] — [1]II. Physikalisches Institut 50937 Köln — [2]Inst. of Sol. State & Semicond. Phys., Minsk

Thermal conductivity of low-dimensional spin systems is investigated because of the possibility of a large magnetic contribution to the heat transport. There is a lot of evidence for such a contribution in various 1D systems, but it is less investigated in 2D systems. We present measurements of the thermal conductivity κ of $SrCuO_2Cl_2$ [1] and R_2CuO_4 with R = Pr, Nd, Sm, Eu and Gd. For all samples, κ is anisotropic with a conventional low-temperature maximum for a heat current perpendicular to the Cu-O-planes, whereas for a heat current within the Cu-O-planes a second high-temperature maximum or shoulder occurs. In principle, two mechanisms could explain a double-peak structure of κ. One is an unusual phonon-damping, which is e.g. relevant in the 2D-System $SrCu(BO_3)_2$ [2]. Such a damping could arise from soft phonon modes caused by structural instabilities. The other is an additional contribution by magnetic excitations of the spin system. However, a structural instability is only present for R=Eu and Gd. Thus, the observation of a double-peak structure in all samples gives clear evidence for a sizeable heat transport by magnetic excitations. We also show, that weak charge-carrier doping strongly suppresses the magnetic contribution.

[1] M. Hofmann et al. PRB 67, 184502 (2003)
[2] M. Hofmann et al. PRL 87, 047202 (2001)
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TT 32.5 Di 17:15 TU H2053

$Sr_2Cu(PO_4)_2$ - an unexpected one dimensional spin 1/2 Heisenberg system with isolated CuO_4 units — •Helge Rosner[1], Michelle Johannes[2], Johannes Richter[3], and Stefan-Ludwig Drechsler[4] — [1]MPI for Chemical Physics of Solids, Dresden — [2]NRL Washington, USA — [3]Otto-von-Guericke-University Magdeburg — [4]Leibniz Institute for Solid State and Materials Research Dresden

Recently, Belik *et. al.* [1] reported synthesis and physical properties of the compound $Sr_2Cu(PO_4)_2$. The measured magnetic susceptibility [1] exhibits a broad maximum at 92 K characteristic for quasi-1D systems, but shows no long range magnetic ordering down to 0.45 K. Here, we present full potential electronic structure calculations within the local spin density approximation, followed by a subsequent mapping to a one-band tight-binding model and an extended Heisenberg model. Although the crystal structure of $Sr_2Cu(PO_4)_2$ is formed by unlinked CuO_4 units, we find a surprisingly pronounced one dimensional behaviour with substantial coupling between nearest neighbors (NN) only. The calculated NN exchange coupling $J_1 \sim 180$ K is in good agreement with the experimental estimate. It exceeds all other couplings by at least two orders of magnitude, placing the system in the forefront of 1D spin 1/2 model compounds. Model calculations using the derived exchange constants suggest that no long range magnetic ordering should be expected down to very low temperatures.

[1] Belik *et. al.*, J. of Sol. Stat. Chem. **177**, 883 (2004).

TT 32.6 Di 17:30 TU H2053

Evidence for bound holes in the doped spin ladders of $(Sr,Ca)_{14}Cu_{24}O_{41}$ — •C. Hilgers[1], M. Grüninger[1], A. Freimuth[1], U. Ammerahl[2,3], P. Ribeiro [4], B. Büchner[4], and A. Revcolevschi[3] — [1]II. Physikalisches Institut, Universität zu Köln — [2]II. Physikalisches Institut, RWTH-Aachen — [3]Laboratoire de Physico-Chimie de L'Etat Solides, Université Paris-Sud, France — [4]IFW Dresden

In the telephone-number compounds $(Sr,Ca)_{14}Cu_{24}O_{41}$ the interplay of spin and charge degrees of freedom gives rise to a competition between charge-density wave (CDW) and superconducting (SC) ground states. Superconductivity was found in $Sr_{14-x}Ca_xCu_{24}O_{41}$ under external pressure for x $\geq$ 11.5, whereas for x $\leq$ 8 a charge ordering in the chains and a CDW ground state in the ladders were observed. However, the nature of the CDW ground state is still unresolved. We present a detailed study of the doping dependence of the optical conductivity in the far-infrared range as a function of temperature and polarization (E$\|$a,c). Between x = 6 and x = 8, we observe a qualitative change of $\sigma_a(\omega)$ and $\sigma_c(\omega)$ with new collective modes for x = 8. We interpret these modes as evidence for bound holes in the ladders. For x $\leq$ 8, we observe a new optical phonon mode at low temperatures which can be attributed to a Raman-active ladder mode activated by the CDW. We report an interesting correlation between transition temperatures of the CDW ground state in the ladders and charge ordering in the chains.

TT 32.7 Di 17:45 TU H2053

Spin chains in (Ca,La,Sr)$_{14}$Cu$_{24}$O$_{41}$ — •Cosima Schuster and Udo Schwingenschlögl — Institut für Physik, Universität Augsburg

The (Ca,La,Sr)$_{14}$Cu$_{24}$O$_{41}$ compounds contain two different structural components, CuO_2 ladders and CuO chains. The compounds are intrinsically doped, whereby the main part of the holes can be assigned to the chains. The spin and charge order on the chains are strongly doping dependent and range from spin dimers over 3D antiferromagnetic order to ferromagnetic order in the La rich compounds. On the basis of the crystal structure we try to form a model for the chains on the basis of the Hubbard model. We choose the Hubbard model, because it is particle-hole-symmetric, and the doping is numerically easy to implement. In addition we study periodic potentials with different period. We examine, which potential is energetically favored and which charge and spin order is linked with this potential. In our investigations we concentrate on the quarter filled band. We find that a $2k_F$ periodic magnetic field leads – with interaction – to the highest energy gain but it is related with a large spin gap. On the other hand a $4k_F$ periodic potential is favored for strong interaction. In this case, we find no spin gap but a $2k_F$ oscillation of the magnetization. The difference to a Heisenberg chain is pointed out.

TT 32.8 Di 18:00 TU H2053

DIMER FORMATION IN THE Cu (S=1/2) SPIN CHAINS OF Sr$_{13}$LaCu$_{24}$O$_{41}$ — •H.-H. Klauss[1], H. Gerdes[1], A. Bosse[1], H.-J. Grafe[1,2], D. Mienert[1], J. Litterst[1], R. Klingeler[2], and B. Büchner[2] — [1]Institut für Metallphysik und Nukleare Festkörperphysik, TU Braunschweig, 38106 Braunschweig — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Helmholtzstr. 20, 01069 Dresden

We present a comparitive ^{63}Cu-NMR study on the Cu chain site in Sr$_{13}$LaCu$_{24}$O$_{41}$ and Sr$_{14}$Cu$_{24}$O$_{41}$. The experiments on the ≈ 60 % hole doped antiferromagnetic (AFM) spin chains in Sr$_{14}$Cu$_{24}$O$_{41}$ confirm the existence of local dimers with a spin excitation gap of $\Delta \approx 130$ K in good agreement with [1]. The formation of weakly interacting dimers is explained by a specific charge order model. In Sr$_{13}$LaCu$_{24}$O$_{41}$ the hole doping is reduced to ≈ 50 %. In a static alternating spin/hole charge order model an AFM S=1/2 spin chain with a gapless Bonner-Fisher behavior is expected. Susceptibility measurements indeed verify the absence of a spin gap. We present NMR experiments which reveal a strongly temperature dependent Knight shift and T_1 relaxation rate below 150 K which can be described by a thermal activation over a finite spin excitation gap. Possible reasons for this discrepancy will be discussed. [1] M. Takigawa et al., PRB 57 (1998) 1124

TT 32.9 Di 18:15 TU H2053

Strong Coulomb effects in hole-doped Heisenberg chains — •Jürgen Schnack — Universität Osnabrück, Fachbereich Physik, D-49069 Osnabrück, Germany

Substances like the “telephone number compound” Sr$_{14}$Cu$_{24}$O$_{41}$ are intrinsically hole-doped. The involved interplay of spin and charge dynamics is a challenge for theory. In this Letter we propose to describe hole-doped Heisenberg spin rings by means of complete numerical diagonalization of a Heisenberg Hamiltonian that depends parametrically on hole positions and includes the screened Coulomb interaction among the holes. It is demonstrated that key observables like magnetic susceptibility, specific heat, and inelastic neutron scattering cross section depend sensitively on the dielectric constant of the screened Coulomb potential which opens the fascinating possibility to determine the in-medium dielectric constant experimentally from such observables [1,2].

[1] J. Schnack, Phys. Rev. Lett., submitted, cond-mat/0409650
[2] J. Schnack, F. Ouchni, J. Magn. Magn. Mater. (2004) accepted, cond-mat/0406592