TT 34 Correlated Electrons: Spin Systems and Itinerant Magnets

Time: Friday 10:15–12:30 Room: HSZ 301

TT 34.1 Fri 10:15 HSZ 301

Nonmagnetic Impurities in the Two-Dimensional Kondo-Necklace — •Wolfram Brenig — Institute for Theoretical Physics, Technical University of Braunschweig, Germany

The effects of nonmagnetic impurities on the two-dimensional spin-1/2 Kondo-necklace model are investigated. In its undoped state this spin-model displays a quantum-critical point at a Kondo-exchange coupling of $J \approx 1.4$ which separates a dimerized singlet-phase from an antiferromagnetically ordered ground state. Using quantum Monte-Carlo calculations based on the stochastic series expansion, results will be presented for the uniform susceptibility and the staggered structure factor as a function of temperature, impurity concentration, and Kondo exchange. It will be shown, that on dilution of the Kondo sites the systems develops quasi-free moments with a renormalized Curie-constant. Moreover, the quantum critical point is suppressed, with a disorder induced long-range antiferromagnetic order to appear also in the singlet phase, which amounts to an order-from-disorder phenomenon.

TT 34.2 Fri 10:30 HSZ 301

Phase diagram of the two-dimensional quantum Heisenberg antiferromagnet with an easy-axis anisotropy — •Martin Holtschneider[1], Stefan Wessel[2], and Walter Selke[1] — [1]Institut für Theoretische Physik, RWTH Aachen — [2]Institut für Theoretische Physik, Universität Stuttgart

The square lattice spin-1/2 Heisenberg antiferromagnet with an easy-axis anisotropy is studied in an external magnetic field, using Quantum Monte Carlo simulations based on the stochastic series expansions with a directed loop update. The model displays long range ordered antiferromagnetic, algebraically ordered spin-flop, and paramagnetic phases. The low-temperature phase diagram is determined by studying both thermodynamic quantities such as the (staggered) suszeptibility and the staggered magnetization as well as histograms of e.g. the order parameter distribution. The numerical results are compared to previous findings on this model (being equivalent to a hard core boson Hubbard model), in particular G. Schmid et al., Phys. Rev. Lett. 88, 167208 (2002), and the results on the corresponding classical model in M. Holtschneider et al., Phys. Rev. B 72, 064443 (2005).

TT 34.3 Fri 10:45 HSZ 301

Reduction of surface coverage of finite systems due to geometrical steps — •C. Olbrich[1], K. Morawetz[1,2], S. Gemming[3], and M. Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [3]Institute of Physical Chemistry, Technical University Dresden, Germany

The coverage of surfaces interrupted by a step with molecules is simulated by a two-dimensional Ising model. An analytical mean-field model is developed which is capable to describe main properties of this frustrated Ising model due to the surface geometry. We find a reduction of coverage (magnetization) at low temperatures due to the presence of the surface step for certain bonding strengths. This represents a second transition besides the usual phase transition and is characterized by a diverging susceptibility and magnetization as a finite-size effect. The specific heat diverges with a power law due to the surface step.

TT 34.4 Fri 11:00 HSZ 301

Evidence for collective orbital excitations in YVO_3 — •E. Benckiser[1,2], R. Rückamp[1], M. Grüninger[2], A.A. Nugroho[3], and T.T.M. Palstra[3] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]II. Physikalisches Institut, RWTH Aachen, Germany — [3]Materials Science Centre, Rijksuniversiteit Groningen, The Netherlands

The compound YVO_3 recently has attracted a lot of interest because of its unusual structural, orbital and magnetic properties [1,2]. The compound undergoes a series of temperature-induced phase transitions accompanied by a change of orbital and magnetic order. Furthermore it has been proposed that YVO_3 represents the first realization of a one-dimensional orbital liquid and an orbital Peierls phase, with a transition to an orbitally ordered phase at lower temperatures [3].

We present the optical conductivity $\sigma(\omega)$ of YVO_3 single crystals for energies from 0.1 eV to 1.6 eV and temperatures from 15 K to 300 K. The data have been collected by performing measurements using linearly polarized light with the electric field vector parallel to the crystallographic axes (σ_a,σ_b,σ_c). The results give clear evidence for orbital excitations. In particular the strong polarization and temperature dependence of two peaks observed at 0.3 eV in σ_c and 0.5 eV in σ_a are hard to reconcile with an interpretation in terms of local crystal-field excitations. We propose an interpretation in terms of orbitons and discuss a simple model describing a two-orbiton absorption process. [1] Ren *et al.*, Nature **396**, 441(1998); [2] Blake *et al.*, PRB **65**, 174112 (2002); [3] Ulrich *et al.*, PRL **91**, 257202 (2003). *Supported by the DFG through SFB 608.*

TT 34.5 Fri 11:15 HSZ 301

Helimagnetism and Weak Ferromagnetism in the Edge-Shared Chain Cuprate $NaCu_2O_2$ — •S.-L. Drechsler[1], J. Richter[2], A.A. Gippius[3], A.N. Vasiliev[3], A.A. Bush[4], A.S. Moskvin[5], J. Malek[6], Yu. Prots[7], W. Schnelle[7], and H. Rosner[7] — [1]IFW-Dresden, 01171 Dresden, PF 270116, Germany — [2]Universität Magdeburg, Germany — [3]Moscow State University, Russia — [4]Moscow Inst. of Radiotechnics, Electronics and Automation, Russia — [5]Ural State University Ekaterinburg, Russia — [6]FZU AVCR, Praha, Czech Rep. — [7]MPI-cPfS Dresden, Germany

We report on susceptibility, magnetization, ^{23}Na NMR, and specific heat data of the spin-chain material $NaCu_2O_2$ in the paramagnetic and ordered phases. Below 13 K, where a sharp field-dependent specific heat peak appears, the NMR lineshape points to an incommensurate static modulation of the local magnetic field consistent with a spiral arrangement of the Cu magnetic moments. At 2 K weak ferromagnetism with a small ordered moment of about $4{\cdot}10^{-3}\mu_B$ has been observed. LDA based estimates of exchange integrals reveal a large inchain frustration leading to a magnetic spiral.

TT 34.6 Fri 11:30 HSZ 301

Itinerant iron magnetism and high spin polarization in filled skutterudites — •Helge Rosner, Andreas Leithe-Jasper, Walter Schnelle, Joerg Sichelschmidt, Steffen Wirth, John Mydosh, and Yuri Grin — MPI CPfS Dresden

Compounds with the filled skutterudite structure are currently under intensive investigation due to their wide spectrum of ground state properties. Here, we report a combined theoretical and experimental study of the electronic and magnetic properties of the compound family AFe_4Sb_{12} (A=Na,K,Ca,Ba,Yb) by means of band structure calculations and measurements of point-contact Andreev reflections, optical spectra and thermodynamic properties (χ, C_P, ρ). Whereas the compounds with A=Na,K order ferromagnetically [1] with a high transport spin polarisation $P_t \sim 67\%$ [2], the magnetic order for A=Ca,Ba,Yb is suppressed by strong spin fluctuations. The latter compounds show a metamagnetic transition in high magnetic fields as suggested by fixed spin moment calculations. The Yb compound, formerly considered as a heavy fermion system, is proven to be in a stable divalent state by band structure calculations and optical and thermodynamic data [3].

[1] A. Leithe Jasper *et al.* Phys. Rev. Lett. **91**, 037208 (2003).
[2] G. Sheet *et al.* Phys. Rev. B **72**, in print (2005).
[3] W. Schnelle *et al.* Phys. Rev. B **72**, 020402(R) (2005).

TT 34.7 Fri 11:45 HSZ 301

Orbital Ordering and Spin-Ladder Formation in La_2RuO_5 — •Volker Eyert, Stefan G. Ebbinghaus, and Thilo Kopp — Institut für Physik, Universität Augsburg

The semiconductor-semiconductor transition of La_2RuO_5 is studied by means of augmented spherical wave (ASW) electronic structure calculations as based on density functional theory and the local density approximation. This transition has lately been reported to lead to orbital ordering and a quenching of the local spin magnetic moment. Our results give strong hints for a different orbital ordering scenario than the one previously proposed. In our type of ordering, the local $S = 1$ moment at the Ru sites is preserved in the low-temperature phase. The unusual magnetic behaviour is interpreted by the formation of spin-ladders, which result from the structural changes occurring at the transition and are characterized by antiferromagnetic coupling along the rungs.

TT 34.8 Fri 12:00 HSZ 301

Investigation of Orbital and Magnetic Order in Ruthenates with Resonant X-ray Diffraction — •Ioannis Zegkinoglou[1], J. Strempfer[1], B. Bohnenbuck[1], C.S. Nelson[2], C. Bernhard[1], and B. Keimer[1] — [1]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]National Synchrotron Light Source, Brookhaven National Laboratory, Upton, USA

Resonant x-ray diffraction at the L_{II} and L_{III}-absorption edges of ruthenium has been used to investigate orbital and magnetic order in $4d$ transition metal oxide single crystals. A large resonance enhancement of the magnetic scattering cross-section due to electric dipole transitions directly into the $4d$ band is observed. In the single-layered Mott transition system Ca_2RuO_4, a new phase transition between two paramagnetic phases is observed around 260 K, at the wave-vector characterizing the low-temperature antiferromagnetic order [1]. Based on the polarization and azimuthal angle dependence of the diffracted intensity, the new phase transition is attributed to the ordering of the Ru t_{2g} orbitals. In $RuSr_2GdCu_2O_8$, the antiferromagnetic order of Ru ions and the possible effect of the onset of superconductivity on it below $T_c \approx 40$ K are investigated. Due to the sensitivity of resonant x-ray diffraction to the azimuthal angle, a precise determination of the direction of the magnetic moment in the system is possible.

[1] I. Zegkinoglou, J. Strempfer et al., Phys. Rev. Lett. 95, 136401 (2005)

TT 34.9 Fri 12:15 HSZ 301

Spin-Orbital Model for Layered Manganites — •Maria Daghofer[1] and Andrzej Oleś[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Jagellonian University Kraków, Poland

We present a spin-orbital t-J model for undoped and doped manganites at $T = 0$ and at finite temperature. The model fully takes into account onsite Coulomb repulsion of these strongly correlated materials. We investigate it by use of Exact Diagonalization and Monte Carlo techniques.

With inclusion of a crystal field term, we obtain a realistic model for $La_{1-x}Sr_{1+x}MnO_4$, showing a gradual change from predominantly out-of-plane $(3z^2 - r^2)$ to more in-plane $(x^2 - y^2)$ orbital occupation both with doping and with rising temperature. At higher doping, we obtain the CE-AF phase for $x = 0.5$ as well as the C-AF phase observed in $Nd_{1-x}Sr_{1+x}MnO_4$ at $x > 0.75$.

For undoped bilayer clusters, we obtain for realistic parameter values the A-AF phase observed in three-dimensional compounds, with orbital correlations in accordance with experiment. At high doping, the model predicts the C-AF and G-phases as they are found in strongly doped $La_{2-2x}Sr_{1+2x}Mn_2O_7$.