TT 12: Correlated Electrons: Spin Systems and Itinerant Magnets 2

Time: Monday 14:00–16:00 Location: HSZ 304

TT 12.1 Mon 14:00 HSZ 304

Systematic derivation of generalized t-J models from Hubbard models away from half-filling — •Simone Hamerla[1] and Götz S. Uhrig[1,2] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, 44221 Dortmund, Germany — [2]School of Physics, University of New South Wales, Kensington 2052, Sydney NSW, Australia

Starting from a fermionic Hubbard model a generalized t-J model is constructed by eliminating charge fluctuations which change the number of double occupancies. The charge fluctuations are eliminated by a systematic change of basis performed by self-similar continuous unitary transformations [1]. The proliferating terms are truncated according to their spatial extension. The derivation of a generalized t-J model is possible as long as the system is dominated by the local repulsion. In the present work, we focus on the Hubbard model on the linear chain and on the square lattice. There are two main goals: one is to test different choices of the infinitesimal generator, the other is to elucidate the influence of doping.

[1] A. Reischl, E. Müller-Hartmann, G. S. Uhrig, Phys. Rev. B 70, 245124

TT 12.2 Mon 14:15 HSZ 304

Dynamic Spin Excitations and Magnetism in the Hubbard Model — •Sebastian Schmitt — Lehrstuhl für Theoretische Physik II, TU Dortmund

The static and dynamic magnetic susceptibility of the Hubbard model is calculated within the dynamical mean field theory (DMFT) using the enhanced non-crossing approximation (ENCA) as impurity solver. The magnetic properties are discussed for various dopings, temperatures and lattices with and without frustration. Special emphasis is laid on the interpretation in terms of the two fundamental pictures of magnetism, i.e. Stoner-type magnetism of itinerant electronic excitations and Heisenberg spin-magnetism of localized magnetic moments. The transition between these two opposing pictures is discussed. An interesting reentrant behavior is observed for the antiferromagnetic Néel temperature in the intermediate coupling region. Additionally, a dispersionless collective mode is observed in the dynamic magnetic susceptibility for large values of the Coulomb repulsion at very low temperatures, indicating a localized singlet-triplet excitation connected with the breakup of local Kondo-singlets.

TT 12.3 Mon 14:30 HSZ 304

The frustrated ferromagnetic $S = 1/2$ Heisenberg chain in a magnetic field – How multipolar spin correlations emerge from magnetically ordered states — Julien Sudan[1], Andreas Lüscher[1], and •Andreas M. Läuchli[2] — [1]IRRMA, EPF Lausanne, Switzerland — [2]MPI für Physik komplexer Systeme, Dresden, Germany

We present the phase diagram of the frustrated ferromagnetic $S = 1/2$ Heisenberg J_1-J_2 chain in a magnetic field, obtained by large scale exact diagonalizations and density-matrix-renormalization-group simulations. A vector chirally ordered state, metamagnetic behavior and a sequence of spin multipolar Luttinger liquid phases up to hexadecupolar order are found. Starting from classical considerations, we point out that various multipolar correlations are imprinted in a magnetic state and that they can survive the onset of frustration and quantum fluctuations which destroy the convention al magnetic order. Our results also shed new light on previously discovered spin multipolar phases in two-dimensional $S = 1/2$ quantum magnets in a magnetic field. We conclude by presenting numerical results on the dynamical spin structure factor in the various phases which are valuable in identifying multipolar phases in experiments.

TT 12.4 Mon 14:45 HSZ 304

Ferromagnetic mixed-spin chain model for $MnNi(NO_2)_4(en)_2$ (en = ethylenediamine) — •Andreas Honecker[1], Wolfram Brenig[2], Stefan Süllow[3], Matthias Bleckmann[3], and Ralf Feyerherm[4] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen — [2]Institut für Theoretische Physik, TU Braunschweig — [3]Institut für Physik der Kondensierten Materie, TU Braunschweig — [4]Helmholtz-Zentrum Berlin für Materialien und Energie

$MnNi(NO_2)_4(en)_2$, en = ethylenediamine contains ferromagnetically coupled chains with alternating spins of magnitude 1 and 5/2. Two energy scales are observed in the field-dependent specific heat of this compound. This behavior is attributed to the existence of an acoustic and an optical mode in the spin wave dispersion. Parameters for a realistic model have been derived from the high-temperature behavior of the magnetic susceptibility.

Here we present numerical results for the specific heat obtained by exact diagonalization and Quantum-Monte-Carlo simulations for the alternating spin chain model. $MnNi(NO_2)_4(en)_2$ orders antiferromagnetically at low temperatures in zero magnetic field, demonstrating relevant antiferromagnetic interchain coupling. This interchain coupling is included in the numerical treatment at the mean-field level.

15 min. break

TT 12.5 Mon 15:15 HSZ 304

Quasiparticle Renormalization of Bulk Conduction Band States in a Ferromagnet at High Binding Energies — •A. Hofmann[1], X. Y. Cui[2], J. Schäfer[1], S. Meyer[1], P. Höpfner[1], L. Patthey[2], E. Rotenberg[3], J. Bünemann[4], F. Gebhard[4], T. Ohm[5], W. Weber[5], and R. Claessen[1] — [1]Physikal. Institut, Universität Würzburg — [2]Paul-Scherrer-Institut, Villigen — [3]Lawrence Berkeley Nat. Laboratory — [4]Universität Marburg — [5]TU Dortmund

Many-body effects in metals can often be captured within the quasiparticle picture, where bare electrons become dressed with bosonic excitations. Angle-resolved photoemission (ARPES) is the probe of choice to detect such energy renormalization. Beyond electron-phonon coupling one expects interaction with spin excitations, which was identified in *surface* states of Fe(110) [1]. For *bulk* states, symmetry planes of k-space yield the desired hole spectral function.

By high-resolution ARPES we have studied the quasiparticle spectra of the ferromagnet Ni for binding energies up to 500 meV. Using a Gutzwiller calculation as reference, we find significant renormalization in the 250-300 meV range, as identified for magnetic bulk bands for the first time. The self-energy is well described within an electron-magnon coupling model, consistent with neutron scattering. The results also relate to a recent theoretical model [2], which describes kinks in correlated systems as transition between different renormalization regimes.

[1] J. Schäfer *et al.*, Phys. Rev. Lett. **92**, 097205 (2004).

[2] K. Byczuk *et al.*, Nature Phys. **3**, 168 (2007).

TT 12.6 Mon 15:30 HSZ 304

Collective spin-excitations in Cu L and O K edge Resonant Inelastic X-ray Scattering from $Sr_{14}Cu_{24}O_{41}$ — •Thorsten Schmitt[1], Justina Schlappa[1], F. Vernay[1], V. Strocov[1], V. Ilakovac[2], B. Thielemann[1], H. Ronnow[1], J. Mesot[1], B. Delley[1], and L. Patthey[1] — [1]Paul Scherrer Institut, Villigen PSI, Switzerland — [2]UPMC, Paris, France

The spin-ladder / spin-chain compound $Sr_{14}Cu_{24}O_{41}$ is a low-dimensional spin system, which is known for its complex interplay between charge and spin degrees of freedom. One of the subsystems is formed by 2-leg ladders Cu_2O_3, which have the properties of a spin liquid with a finite spin gap [1]. Resonant inelastic X-ray scattering (RIXS) is a powerful probe of the electronic ground state and the low-energy excitation spectrum of transition-metal oxides, being directly sensitive to the valence electron configuration [2]. Using RIXS at the Cu L_3 and O K edge of $Sr_{14}Cu_{24}O_{41}$ [1,2] we observe collective spin-excitations from the ladders, which we assign to two-triplon modes [3]. At the Cu L_3 resonance the dispersion of the modes was mapped out depending on the momentum transfer with excellent sensitivity over almost the entire first Brillouin-zone, in contrast to inelastic neutron scattering [4]. Site-sensitive RIXS at the O K edge of the chain- and ladder-subsystems give insight into the character of the holes.

[1] T. Vuletic et al., Physics Reports 428, 169-258 (2006).

[2] A. Kotani and S. Shin, Rev. Mod. Phys. 73, 203 (2001).

[3] K. P. Schmidt and G. S Uhrig. Mod. Phys. Rev. Lett. 90, 227204 (2003).

[4] S. Notbohm et al., Phys. Rev. Lett. 98, 027403 (2007).

TT 12.7 Mon 15:45 HSZ 304

Orbitons and bi-orbitons in YVO_3 — •Luis Mäder[1], Eva Benckiser[1,2], Giacomo Ghiringhelli[3], Marco Moretti[3], Graeme

R. Blake[4], Nandang Mufti[4], A. Agung Nugroho[4,5], Thomas T. M. Palstra[4], Maurits Haverkort[2], and Markus Grüninger[1] — [1]Universität zu Köln — [2]MPI-FKF Stuttgart — [3]Politecnico di Milano — [4]University of Groningen — [5]Institut Teknologi Bandung

The aim of the project is the unambiguous observation of a novel kind of elementary excitations in a solid, namely orbitons, propagating orbital excitations. In an orbitally ordered state, one expects that exchange interactions between orbitals on neighbouring sites give rise to a significant dispersion of the orbital excitations. These orbitons are analogous to spin waves in a magnetically ordered state.

Orbital exchange interactions are expected to be strong in the Mott insulator YVO_3.

Here, we report on the observation of orbital excitations in YVO_3 by means of high-resolution resonant inelastic x-ray scattering (RIXS) across the V $L_{3,2}$ (V $2p \rightarrow$ V $3d$) and O K (O $1s \rightarrow$ O $2p$) edges with the new SAXES beamline at the PSI, Villigen. Due to the excellent resolution of 60-70 meV, we are able to resolve the intra-t_{2g} excitations, spin-flip excitations within the t_{2g} shell, and excitations into the e_g levels, in excellent agreement with our recent optical data [1]. Moreover, we find evidence for a bi-orbiton excitation. Finally, our data show that SAXES in principle should allow to study the orbital excitations as a function of the wave vector k.

[1] E. Benckiser *et al.*, New J. Phys. **10**, 053027 (2008).