TT 27: CE: Poster Session

Time: Wednesday 14:00–18:00 Location: Poster D1

TT 27.1 Wed 14:00 Poster D1

Soft-Mode Behaviour of Phonons in the CDW Systems $NbSe_2$ and $TiSe_2$ — •Roland Hott[1], Rolf Heid[1], Klaus-Peter Bohnen[1], Frank A. Weber[2], Stephan Rosenkranz[2], John-Paul A. Castellan[2], and Ray Osborn[2] — [1]Karlsruhe Institute of Technology, Institut für Festkörperphysik, P.O.Box 3640, D-76021 Karlsruhe — [2]Neutron & X-ray Scattering Group, Materials Science Division, Argonne National Laboratory, 9700 S Cass Ave, Argonne, IL, 60439

We investigated the soft-mode behaviour of phonons in the CDW systems $NbSe_2$ and $TiSe_2$ both theoretically in DFT-based ab-initio phonon calculations and experimentally by means of X-ray scattering. For $NbSe_2$, our calculations predict the development of a phonon instability on reduction of the thermal broadening of the electronic states, in good agreement with the experimental findings. For $TiSe_2$, our theoretical description correctly indicates a softening of the phonon dispersions in the experimentally observed critical regions of the Brillouin zone. However, the effect predicted here by our DFT-description appears to be too weak to explain the experimentally observed CDW instability.

TT 27.2 Wed 14:00 Poster D1

Dilatometric Investigations at the Charge-Ordering Transition in $(TMTTF)_2X$ — •Daniel Hofmann[1], Mariano de Souza[1], Christian Balz[1], P. Foury-Leylekian[2], A. Moradpour[2], J.-P. Pouget[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität, Max-von-Laue Str. 1, SFB/TR49 D-60438 Frankfurt (M), Germany — [2]Laboratoire de Physique des Solides, Université Paris Sud, CNRS UMR 8502, Orsay, France

We report results of high-resolution measurements of the c^*-axis expansivity (α_{c^*}) at the charge-ordering (CO) transition for the quasi-1D $(TMTTF)_2X$ compounds with X = Br and SbF_6 and make a comparison with previous results for the X = PF_6 and AsF_6 salts [1]. For X = SbF_6, due to the screening of the long-range Coulomb forces, a sharp λ-type anomaly is observed at T_{CO}, which contrasts with the step-like mean-field anomaly at T_{CO} for PF_6 and AsF_6, where CO occurs in the Mott-Hubbard charge-localized regime. For the latter two salts, a negative contribution to α_{c^*} is observed above T_{CO}. This effect is assigned to the anions' rigid-unit modes, which become inactive for $T < T_{CO}$. Measurements for the X = Br salt, where such rigid-unit modes are absent, reveal no traces of such negative contribution to α_{c^*}, confirming the model based on the anions' rigid-unit modes for the X = PF_6 and AsF_6 salts [1].

[1] M. de Souza *et al.*, Phys. Rev. Lett. **101**, 216403 (2008).

TT 27.3 Wed 14:00 Poster D1

Energy gap in charge-density-wave systems — •Reinhard Rossner[1], Hans-Martin Eiter[1], Michela Lavagnini[2], Leonardo Tassini[1], Bernhard Muschler[1], Jiun-Haw Chu[3], Nancy Ru[3], Ian R. Fisher[3], Leonardo Degiorgi[2], and Rudi Hackl[1] — [1]Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, D-85748 Garching, Germany — [2]Laboratorium für Festkörperphysik, ETH - Zürich, CH-8093 Zürich, Switzerland — [3]GLAM, Stanford University, Stanford, California 94305, USA

The rare-earth tri-tellurides show a phase transition to a charge-density-wave ground state, some of them at temperatures well above 300 K. As a consequence an energy gap Δ opens up. We observed this gap in $DyTe_3$ and $LaTe_3$ by measuring the electronic Raman effect as a function of polarization in the temperature range from 6 K to 311 K. The gap becomes more pronounced with decreasing temperature. The magnitudes of Δ are in agreement with those obtained by other experimental techniques such as angle-resolved photoemission spectroscopy. The polarization dependence allows us to study the anisotropy of the gap.

TT 27.4 Wed 14:00 Poster D1

X-ray absorption of hole-doped and electron-doped $Pr_{1-x}Ca_xMnO_3$: Doping-dependent transfer of spectral weight — •Stephan Uebe[1,2], Andrea Assmann[1,2], Michael Merz[1], Prabir Pal[3], Manas Dalai[3], Biju Sekhar[3], Hilbert von Löhneysen[1,2], Peter Nagel[1], and Stefan Schuppler[1] — [1]Karlsruhe Institute of Technology, Institut für Festkörperphysik, Germany — [2]Karlsruhe Institute of Technology, Physikalisches Institut, Germany — [3]Institute of Physics, Bhubaneswar, India

Transition metal oxides like the manganites have intriguing physical properties, many of which are based on unusual interrelations between spin, charge, and orbital degrees of freedom. To better understand the phenomena of charge/orbital ordering (CO/OO) and to possibly isolate the fundamental properties which serve as a driving force for CO/OO we have investigated $Pr_{1-x}Ca_xMnO_3$ with temperature-dependent near-edge x-ray absorption spectroscopy. With respect to CO/OO, $Pr_{1-x}Ca_xMnO_3$ becomes especially interesting since it is a narrow band system with almost identical radii of Pr^{3+} and Ca^{2+}. Changes in the tolerance factor can, therefore, directly be attributed to the t_{2g} and e_g orbital occupation. The present data clearly show that the spectral weight and, thus, the number of unoccupied states near the Fermi energy directly tracks the Ca doping level x. A small but distinct redistribution with temperature between the t_{2g} and e_g states at E_F is observed. Implications of the spectroscopic data will be discussed.

TT 27.5 Wed 14:00 Poster D1

EELS-study of $La_{1-x}Sr_{1+x}MnO_4$ — •Matthias Schrade, Roberto Kraus, Pascal Reutler, Jochen Geck, Martin Knupfer, and Bernd Büchner — Institute for Solid State Research, IFW Dresden

The layered manganite $La_{1-x}Sr_{1+x}MnO_4$ displays a strong interplay of charge-, spin-, and orbital degrees of freedom, which results in complex electronic properties.

We performed a detailed electron energy loss spectroscopy (EELS) study in order to clarify the charge dynamics in these materials as a function of doping and temperature.

A new feature at 1.8 eV rapidly gains spectral weight with increasing x. This low energy excitation shows little dispersion, but for $x > 0.25$ an additional excitation appears around 1 eV for high q-values.

At low T, the magnetic superstructure for half doping could be observed, coinciding with a 0.3 eV-shift of the 1.8 eV-excitation. An interpretation of the physical origin of the different excitations will be proposed.

TT 27.6 Wed 14:00 Poster D1

Orbitons and bi-orbitons in $GdVO_3$ and YVO_3 observed by RIXS — •Luis Mäder[1], Komalavalli Thirunavukkuarasu[1], Eva Benckiser[2,1], Giacomo Ghiringhelli[3], Marco Moretti[3], Graeme R. Blake[4], Nandang Mufti[4], Agung A. Nugroho[5,4], Thomas T. M. Palstra[4], Maurits Haverkort[2], Thorsten Schmitt[6], and Markus Grüninger[1] — [1]Universität zu Köln — [2]MPI-FKF Stuttgart — [3]Politecnico di Milano — [4]University of Groningen — [5]Institut Teknologi Bandung — [6]PSI, Villigen

In an orbitally ordered state, one expects that exchange interactions between orbitals on neighbouring sites give rise to a novel kind of elementary excitations, so called orbitons, which are analogous to spin waves in a magnetically ordered state.

Here, we report on the observation of orbital excitations in YVO_3 and $GdVO_3$ 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 meV, we are able to resolve two different features in the low energy regime. We interpret them as one- and bi-orbiton excitations in good agreement with our optical data [1]. We compare our data with results on $YTiO_3$ and $LaTiO_3$ by Ulrich et al. [2], who attribute the spectral weight at low energies mainly to bi-orbiton excitations.

[1] E. Benckiser *et al.*, New J. Phys. **10**, 053027 (2008).
[2] C. Ulrich *et al.*, PRL **103**, 107205 (2009).

TT 27.7 Wed 14:00 Poster D1

HAXPES analysis of $LaAlO_3/SrTiO_3$ thin films grown under various oxygen partial pressures — •Florian Pfaff[1], Andreas Müller[1,3], Götz Berner[1], Wolfgang Drube[2], Michael Sing[1], and Ralph Claessen[1] — [1]Experimentelle Physik IV, University of Würzburg — [2]HASYLAB DESY, Hamburg — [3]Inorganic Materials Science, University of Twente

At the interfaces of epitaxially grown oxide heterostructures novel phases with unexpected properties may be generated. E.g., for $LaAlO_3/SrTiO_3$ (LAO/STO) a quasi-2DEG is found, if more than four monolayers (ML) of LAO are grown on STO. As possible explanations intrinsic, i.e. electronic reconstruction, but also extrinsic effects like oxygen vacancies are discussed. To analyze the influences of oxygen vacancies, we performed hard x-ray photoelectron spectroscopy (HAXPES) measurements on samples with two and five ML LAO grown under various oxygen partial pressures (10^{-5} mbar, 10^{-3} mbar, and 10^{-1} mbar) by pulsed laser deposition (IMS, U Twente). We used angle-dependent HAXPES on the Ti $2p$ core level to determine the Ti^{3+}/Ti^{4+} ratio, which clearly depends on the growth pressure. Unexpectedly, the five ML sample grown at 10^{-1} mbar - a pressure for which oxygen vacancies should be largely suppressed - shows no Ti^{3+} at all, which is in agreement with its insulating behavior observed in transport measurements, but casts electronic reconstruction as only possible origin for the 2DEG formation into doubt. However, other explanations for the insulating behavior could be involved, like an increased interface roughness or possible Sr-La intermixing.

TT 27.8 Wed 14:00 Poster D1

Preparation and characterization of $PdCoO_2$ thin films grown by Pulsed Laser Deposition — •Stefan Hirsch, Philipp Komissinskiy, and Lambert Alff — TU Darmstadt, Materialwissenschaft, Darmstadt, Deutschland

$PdCoO_2$ has a hexagonal delafossite crystal structure with the lattice constants of $a = 2.83$ Å and $c = 17.74$ Å, and a low resistivity of 4.7 $\mu\Omega$cm perpendicular to the c-axis at 260 K [1]. The aforementioned property is unusual for an oxide material and makes it interesting for thin film applications as an electrode in epitaxial all-oxide heterostructures.

The thin films were produced by pulsed laser deposition (PLD). Single crystals of $PdCoO_2$ were synthesised out of $PdCl_2$ and CoO in evacuated silica tubes. The crystals were grinded, pressed and sintered to a cylindrical pellet to obtain a target for the PLD process. The growth mechanism of the thin films on single crystal substrates was monitored by reflection high energy electron diffraction (RHEED). The thin films were characterized by X-ray diffraction, atomic force microscopy, magnetisation and resistivity measurement from 4.2 to 300 K.

The authors thank DFG GK 1035.

[1] M.Tanaka et al., J. Physical Society of Japan 65, 3973 (1996)

TT 27.9 Wed 14:00 Poster D1

Superconductivity in the hybrid dichalcogenide 18R-$SnSe_2\{CoCp_2\}_x$ — •Michael Herzinger, Robert Miller, Sandra Altmannshofer, Ernst–Wilhelm Scheidt, and Wolfgang Scherer — Lehrstuhl für Chemische Physik und Materialwissenschaft, Institut für Physik, Universität Augsburg, 86159 Augsburg, Germany

We report on electronical and thermodynamical properties of the superconducting hybrid materials 18R-$SnSe_2\{CoCp_2\}_x$ ($0 < x < 0.25$). These materials were synthesized by intercalation of the host layered dichalcogene $SnSe_2$ with the organometalic compound cobaltocene ($CoCp_2$).

These materials indicate a highly anisotropic superconducting behavior, which is observed in resistivity as well as susceptibility measurements parallel and perpendicular to the $SnSe_2$-layers. This is also reflected in the coherence length ratio, e.g. for 18R-$SnSe_2\{CoCp_2\}_{0.1}$, perpendicular to the layers of $\xi_\perp(0) = 7$ Å and parallel $\xi_{||}(0) = 717$ Å.

This study was done for different $CoCp_2$-concentration and demonstrates a quasi two-dimensional superconductor with designable physical properties depending on the degree of intercalation.

TT 27.10 Wed 14:00 Poster D1

Hard x-ray photoemission spectroscopy on $LaAlO_3/LaNiO_3$ multilayers — •Patrick Helmecke[1], Götz Berner[1], Michael Sing[1], Johannes Walde[1], Eva Benckiser[2], Georg Cristiani[2], Hanns-Ulrich Habermeier[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universiät Würzburg — [2]MPI-FKF Stuttgart

Recently, oxide heterostructures attract attention due to novel physical properties at their interfaces. A case in point is the 1/1 heterostructure LaO-NiO_2-LaO-AlO_2 (LAO/LNO/LAO). For that it has recently been predicted that by substrate-imposed strain one of the two conductions bands can be pushed up such that it is almost completely depleted. Inclusion of electron-electron interactions would shift this band further up, inducing a single Fermi surface (FS) sheet which resembles that of the high-T_c superconducting cuprates with prospects to carry high-temperature superconductivity as well [1].

While experimentally it is not yet possible to fabricate the 1/1 heterostructure with the required precision, we analyzed multilayers with layer thicknesses between 2uc and 4uc by means of hard-x-ray photoelectron spectroscopy to access the buried LNO layers. Interestingly, from Ni core-level spectra we have found evidence for a charge-transfer in the 2uc/2uc sample to Ni which might have an important impact on the FS topology and hence the idea to artificially design a cuprate-like FS.

[1] P. Hansmann, X. Yang, A. Toschi, G. Khaliullin, O. K. Andersen, and K. Held, Phys. Rev. Lett. 103, 016401 (2009).

TT 27.11 Wed 14:00 Poster D1

Single crystal growth of $CeNi_2Ge_2$ using floating zone technique — •Christoph Bergmann[1], H. S. Jeevan[1], Christoph Geibel[2], and Philipp Gegenwart[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [2]Max-Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany

$CeNi_2Ge_2$ is a well-known paramagnetic moderate heavy fermion compound with the electronic specific heat $\gamma \approx 350$ mJ/K^{2}mol. It shows pronounced non-Fermi liquid behavior, which could be related to a nearby anti-ferromagnetic quantum critical point. Similar to its homologue compound $CeCu_2Si_2$, $CeNi_2Ge_2$ displays a strong sensitive of its low-temperature physical properties to tiny changes in the composition in its physical properties, possibly due to site interchange of Ni and Ge. Aiming to determine the fermi surface, we have grown single crystals of $CeNi_2Ge_2$ using a floating-zone technique. We prepare the feed rod of $CeNi_2Ge_2$ using induction melting or arc melting methods. With these methods we got good quality of single crystals and try to increase the residual resistivity ratio by varying the initial composition. Here we will discuss the relation between the single crystal growth conditions for our floating zone technique, the initial composition and the properties of the obtained single crystal especially their residual resistivity ratio. Additionally we have grown and investigated a crystal with 20% Pd doping to get an anti-ferromagnetic ground state.

Work supported by DFG through SFB 602 and research unit "Quantum phase transitions".

TT 27.12 Wed 14:00 Poster D1

Magnetic anisotropy of flux-grown of $CeAu_2Ge_2$ — •Veronika Fritsch[1], Gerda Fischer[1], Peter Pfundstein[2], Bernd Pilawa[1,3], and Hilbert v. Löhneysen[1,3] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Laboratorium für Elektronenmikroskopie, 76131 Karlsruhe, Germany — [3]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76131 Karlsruhe, Germany

$CeAu_2Ge_2$ crystallizes in the well-known tetragonal $ThCr_2Si_2$ structure. Although the high anisotropy of this crystal structure is often reflected in its magnetic properties, most previous investigations were performed on polycrystals. We succeeded in the growth of $CeAu_2Ge_2$ single crystals in Au-Ge flux as well as in Sn flux. X-ray powder diffraction measurements and EDXS measurements indicate that in the latter case Sn atoms from the flux are incorporated in the samples. We present measurements of the magnetization M demonstrating a strong dependence of the magnetic properties on the flux employed: $M(B)$ curves with the field B aligned along the easy axis in the temperature regime of magnetic order ($T_N = 14.4$ K) reveal with decreasing temperature an increasing number of metamagnetic-like transitions in the Au-Ge-flux grown sample, but only a single one (with increasing field) or two (with decreasing field) metamagnetic-like transitions in the Sn-flux grown sample. With the magnetic field aligned along the hard axis no indication of magnetic order is found in the $M(T)$ curves for small B, where the $M(T)$ curves for the easy axis show a sharp maximum.

TT 27.13 Wed 14:00 Poster D1

Sample preparation and magnetic properties of $CeTiGe_3$ — •Wolfram Kittler[1], Gerda Fischer[1], Veronika Fritsch[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76131 Karlsruhe, Germany

$CeTiGe_3$ crystallizes in the hexagonal $BaNiO_3$-structure (space group $hP10 - P6_3/mmc$), which is also known as hexagonal perovskite. We prepared polycrystals by conventional argon-arc melting with subsequent annealing and quenching in liquid nitrogen. The x-ray powder diffraction patterns showed no traces of impurity phases in our samples, however small deviations from the Curie-Weiss law might be attributed to some impurities still present in the sample. We present measurements of magnetization and electrical resistivity in the temperature range between 1.5 and 300 K in magnetic fields up to 5 T. The resistivity ratio at $T = 1.5$ K of $RRR = 26$, in comparison to the previously reported value of approximately 13 [1], confirms the rather good quality of our samples. The magnetization data show that $CeTiGe_3$ is one of the rare ferromagnetic dense Kondo-lattice compounds with a Curie temperature of $T_C = 14$ K and direction-average magnetic moment of 0.94 μ_B as inferred from the $M(B)$ curves at $B = 5$ T for $T = 5$ K.

[1] P. Manfrinetti et al., Solid State Commun. **135**, 444 (2005).

TT 27.14 Wed 14:00 Poster D1

Electron spin resonance of the Yb $4f$-moment in $Yb(Rh_{1-x}Co_x)_2Si_2$ — •Thomas Gruner, Jörg Sichelschmidt, Christoph Klingner, Cornelius Krellner, Christoph Geibel, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

We present a detailed electron spin resonance (ESR) study on a series of single crystals $Yb(Rh_{1-x}Co_x)_2Si_2$ with Cobalt concentrations x from 0 to 1. All compositions show well defined ESR spectra which can be ascribed to a bulk Yb^{3+} resonance. The pure system $YbRh_2Si_2$ is located in the vicinity of an antiferromagnetic quantum critical point. The magnetic ordering of this system ($T_N = 72$ mK) is stabilized by pressure as it is expected for Yb-Kondo lattice compounds. Doping with Cobalt corresponds to applying chemical pressure. Accordingly, the Néel-temperature is increased to $T_N = 1.7$ K in the pure system $YbCo_2Si_2$, confirming a decrease of the hybridization between conduction electrons and Yb^{3+} $4f$-spins. The anisotropies of the ESR g-factor and the ESR linewidth ΔB for three different frequencies (L, X, Q-band) and in a temperature range from $T \approx 1.5$ K to ≈ 10 K are presented and discussed here. A significant decrease of the anisotropy from $x = 0$ to 1 is observed.

TT 27.15 Wed 14:00 Poster D1

Low-temperature magnetization measurements on $Yb(Rh_{0.93}Co_{0.07})_2Si_2$ — •Luis Pedrero, Manuel Brando, Cornelius Krellner, Christoph Geibel, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

In the heavy-fermion compound $Yb(Rh_{0.93}Co_{0.07})_2Si_2$ a detailed study of the thermodynamic and transport properties at low temperature has shown that the energy scale $T^*(H)$, associated with the Fermi surface reconstruction, vanishes inside the magnetic phase $T_N(H)$, where $T_N = 0.4$ K at zero field [1]. This discovery raises questions as (i) which energy scale is more relevant for quantum criticality in this system, (ii) where are located the strongest signatures of quantum fluctuations (at the critical field of T^* or of T_N) and (iii) which is their intrinsic nature.

To get more insights, we have performed several isofield $M(T)$ and isothermal $M(H)$ magnetization measurements on a high-quality single crystal of $Yb(Rh_{0.93}Co_{0.07})_2Si_2$, to obtain a magnetization grid $M(T, H)$ across the magnetic phase diagram. According to the definition of the Grüneisen ratio $\Gamma_H = -(dM/dT)_H/C_H$ and the Maxwell relation $(dM/dT)_H = (dS/dH)_T$ we could then map the entropy $S(H)$ in and outside the magnetic phase and - supported by specific heat measurements - analyse the divergence of $\Gamma_H(T)$ at both critical fields for T^* and T_N. A direct comparison with the theory will be presented.

[1] S. Friedemann *et al.*, Nat. Phys. **5** (2009) 465.

TT 27.16 Wed 14:00 Poster D1

Low-T magnetic phase diagram of $Yb(Rh_{0.73}Co_{0.27})_2Si_2$ — •Stefan Lausberg[1], Christoph Klingner[2], Cornelius Krellner[1], Manuel Brando[1], Christoph Geibel[1], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Physics Department E14, TU München, James-Franck Str., 85748 Garching, Germany

The heavy fermion system $YbRh_2Si_2$ is situated close to a quantum critical point. At $T_N = 70$ mK it shows a transition to an antiferromagnetic (AFM) phase. Under pressure T_N increases and a second AFM phase emerges at a temperature $T_L < T_N$. Both phases persist up to 8 GPa [2]. Isoelectronic substitution of Rh by Co leads to a similar effect as pressure, apart from the fact that at a Co concentration of 27 % both transition temperatures seem to merge [3].

In this contribution we present low-temperature ac-susceptibility $\chi'(T, H)$ and resistivity $\rho(T, H)$ measurements of high-quality single crystals of $Yb(Rh_{0.73}Co_{0.27})_2Si_2$. We observe just a single magnetic transition in zero field down to 20 mK, which is of the 2^{nd} order. Increasing the field T_N is suppressed at about $\mu_0 H_c \approx 0.53$ T where the phase boundary line drops very rapidly. This suggests that the phase line could become 1^{st} order although no hysteresis is seen at H_c. Furthermore we observe Fermi liquid behavior around the critical field and within the AFM phase.

[1] S. Mederle *et al.*, JMMM **226-230** (2001) 254-255
[2] G. Knebel *et al.*, JPSJ **75** (2006) 114709
[3] C. Klingner, Diploma Thesis (2009), Dresden.

TT 27.17 Wed 14:00 Poster D1

Far-infrared optical conductivity of $CeCu_2Si_2$ — •Alexander Herzog[1], Jörg Sichelschmidt[1], Shin-ichi Kimura[2], Christoph Geibel[1], Hirale Jeevan[1], and Frank Steglich[1] — [1]MPI Chem. Physik fester Stoffe, 01187 Dresden — [2]UVSOR, Institute for Molecular Science, Okazaki 444-8585, Japan

We investigated the optical reflectivity of a S/A-type single crystal of the heavy-fermion metal $CeCu_2Si_2$ in the energy range 3 meV – 30 eV for temperatures between 8K – 300K. Our preliminary results for the charge dynamics indicate a behavior that is expected for a formation of a coherent heavy quasiparticle state [1]: Upon cooling we observe a narrowing of the Drude-like part of the optical conductivity corresponding to an enhancement of the quasiparticle effective mass and scattering time. Furthermore, towards cooling down to $T = 8$ K a redistribution of spectral weight occurs essentially from the energy region below 0.6 eV towards energies below 3 meV.

[1] L. Degiorgi, Rev. Mod. Phys. **71**, 687 (1999)

TT 27.18 Wed 14:00 Poster D1

In situ preparation of $CeIn_3$ thin films by co-sputtering — •Alexander Zaitsev[1], Andre Beck[1], Rainer Fromknecht[1], Markus Wissinger[1], Rudolf Schneider[1], Jochen Geerk[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe

Thin films of the heavy fermion material $CeIn_3$ were prepared in situ on 10x30 mm^2 r-cut sapphire substrates by simultaneous dc sputtering of two stoichiometric $CeIn_3$ targets and dc sputtering of a pure In target in argon gas. The sputtering power of 40 W at each $CeIn_3$ target and 400 W at the In target allowed the deposition of ∼0.5 μm thick $CeIn_3$ films within 40 seconds on the substrate held at 500-550 °C. The resultant films were continuous, smooth and stoichiometric as measured by EDX, although sparse In outgrowths of ∼1 μm size were also observed. According to XRD analysis the films were predominatly (111) oriented, with minor amount of (100) and (110) oriented phases. The dependence of the electrical resistivty on temperature was typically that of bulk $CeIn_3$ with a clear maximum at around 50 K, followed by a linear decrease of resistivity towards lower temperatures. At 10 K a kink in ρ(T) indicated the antiferromagnetic ordering of $CeIn_3$. The residual resistivity ratio $\rho(50K)/\rho(1.4K) = 3$ was reasonably high for the textured thin film material.

TT 27.19 Wed 14:00 Poster D1

Anisotropy in the microwave conductivity of UNi_2Al_3 — •Katrin Steinberg[1], Marc Scheffler[1], Martin Dressel[1], and Martin Jourdan[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany

In the heavy-fermion compound UNi_2Al_3, the free charge carriers show an enhanced effective mass at low temperatures due to electronic correlations. This mass enhancement and a strongly enhanced scattering time can be observed in the microwave conductivity spectrum. The frequency dependent complex conductivity shows a Drude roll-off at a few GHz. From directionally dependent dc studies it is known that UNi_2Al_3 exhibits a pronounced transport anisotropy at low temperatures. To resolve whether the conductivity at microwave frequencies is anisotropic as well, we have prepared strip-shaped thin-film samples of UNi_2Al_3 and measured their conductivity in a broadband microwave Corbino spectrometer with the current parallel to the a-axis or to the c-axis of the hexagonal crystal structure. We present the frequency- and temperature-dependent microwave conductivity (45 MHz to 40 GHz and 1 K to 300 K, respectively) of UNi_2Al_3. The conductivity

spectra exhibit clear Drude roll-offs in both crystallographic directions. They are anisotropic, in consistence with the dc transport. From the measured spectra we obtain the effective mass and scattering rate for both crystal axes and we study their temperature dependence.

TT 27.20 Wed 14:00 Poster D1

Equivalence of pressure and concentration tuning in $CeCu_{6-x}Au_x$ — •O. Stockert[1], A. Hamann[2], V. Fritsch[2], A. Schneidewind[3], and H. v. Löhneysen[2] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Joint Research Group Helmholtz-Zentrum Berlin - Technische Universität Dresden, FRM-II, Garching, Germany

In the prototypical heavy-fermion system $CeCu_{6-x}Au_x$ two different quantum critical scenarios are discussed: the conventional spin-density-wave (SDW) scenario introduced by Hertz, Millis and Moriya and the local scenario by Schröder, Coleman, Si. While concentration and pressure tuning the quantum phase transition (QPT) are described by the local critical scenario, magnetic field tuning the QPT results in the conventional SDW scenario. In order to study how far the analogy between Au substitution and hydrostatic pressure holds, we performed elastic neutron scattering experiments on single crystalline $CeCu_{5.5}Au_{0.5}$ and investigated the magnetic structure under hydrostatic pressure. At a pressure of $p = 8$ kbar the Néel temperature and the propagation vector of the magnetic structure attain almost the values of $CeCu_{5.7}Au_{0.3}$. This concentration-pressure analogy away from the QPT is highly remarkable, since the ambient-pressure magnetic structures of $CeCu_{5.5}Au_{0.5}$ and $CeCu_{5.7}Au_{0.3}$ are quite different. The change of the magnetic structure of $CeCu_{5.5}Au_{0.5}$ under pressure appears to be of first order and to be determined by slight changes in the nesting properties of the Fermi surface. We will discuss our findings in comparison to the different QPTs in the system $CeCu_{6-x}Au_x$.

TT 27.21 Wed 14:00 Poster D1

Luttinger-Ward functional approach in the Eliashberg framework : A systematic derivation of scaling for thermodynamics near a quantum critical point — •Adel Benlagra[1], Ki-Seok Kim[2], and Catherine Pépin[3] — [1]Institut für Theoretische Physik, Universität zu Köln, Germany — [2]Institut de physique Théorique, CEA Saclay, France — [3]Pacific Center for Theoretical Physics, POSTECH, Pohang, South Korea

The poster by Duc-Anh Le et. al. originally scheduled for TT 27.21 has been withdrawn and was replaced by this poster.

We used the Luttinger-Ward (LW) functional in the Eliashberg framework to derive scaling expressions for the free energy from a microscopic model for two models of quantum criticality : the standard theoretical framework called the Hertz-Moriya-Millis theory and the Kondo breakdown model, one possible scenario for heavy-fermion quantum transitions, for which the effective theory is given by a U(1) gauge theory.

The LW functional approach allows to take into account the fluctuation corrections in a systematic way. The Eliashberg framework allows to use the proper level of approximation to get, self-consistently, the correct scaling for thermodynamics near the quantum critical point. We have shown that, at the one loop level, the fermionic excitations give a Fermi Liquid contribution whereas the singular part of the free energy for both models is due to the collective bosonic excitations. In particular, the Kondo breakdown QCP is characterized by two length scales : one is the correlation length for hybridization fluctuations, and the other is that for gauge fluctuations, analogous to the penetration depth in superconductors.

TT 27.22 Wed 14:00 Poster D1

Spin density wave quantum phase transition in the $LuFe_2Ge_2/YFe_2Ge_2$ system — •Zhuo Feng and Malte Grosche — Quantum Matter Group, Cavendish Laboratory, J J Thomson Avenue, Cambridge, CB3 0HE, U.K.

In intermetallic transition metal compounds, spin density wave order and studies of the associated quantum critical point are still comparatively rare. $LuFe_2Ge_2$ has been reported to exhibit spin density wave order below 9K, and its isoelectronic sister compound YFe_2Ge_2 is paramagnetic. Together, they form an attractive system for probing spin density wave quantum criticality. We have grown high quality crystals of YFe_2Ge_2 and $LuFe_2Ge_2$ using flux as well as radio frequency induction methods. YFe_2Ge_2 exhibits an unusually high Sommerfeld coefficient of the specific heat capacity C/T at 1 K in excess of 100 mJ/(molK^2) and still rising significantly with decreasing temperature, as well as an anomalous temperature dependence of the electrical resistivity, $\rho \sim T^{3/2}$. High-pressure measurements are under way in $LuFe_2Ge_2$, to investigate its magnetic phase diagram near the magnetic quantum phase transition, and to examine the associated quantum critical behaviour.

TT 27.23 Wed 14:00 Poster D1

Ferromagnetic quantum phase transition in $Sr_{1-x}Ca_xRuO_3$ thin films — •Melanie Schneider[1], Vasile Moshnyaga[1], Philipp Gegenwart[1], Markus Wissinger[2], and Dirk Fuchs[2] — [1]I. Physikalisches Institut, Georg-August Universität Goettingen,Friedrich-Hund-Platz 1, 37077 Goettingen, Germany — [2]Karlsruher Institut für Technologie (KIT), Institut für Festkörperphysik, Postfach 3640, 76021 Karlsruhe, Germany

We report results on $Sr_{1-x}Ca_xRuO_3$ thin films which have been grown epitaxially on $SrTiO_3$ substrates by metalorganic aerosol deposition. The films are characterized using X-ray diffraction, room-temperature STM, as well as atomic-resolution transmission electron microscopy. The physical properties are investigated by electrical resistivity and magnetization measurements. We observe a continuous suppression of itinerant electron magnetism with T_C=160K for $SrRuO_3$ with increasing Ca concentration x in $Sr_{1-x}Ca_xRuO_3$ towards $T_C \to 0$ for x_c=0.7. At x>0.7 indications for non-Fermi liquid behavior are found in the low-temperature resistivity. For selected thin films the measurements are extended to mK temperatures. We also report low-temperature electrical resistivity measurements on thin films grown at KIT Karlsruhe by pulsed-laser deposition on various different substrates. Work supported by DFG through SFB 602, TP A19.

TT 27.24 Wed 14:00 Poster D1

Low temperature magnetoresistance of different strongly correlated metals close to a quantum phase transition — •M. Schubert, K. Winzer, M. Schneider, H.S. Jeevan, and P. Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

We report measurements of the electrical resistance at temperatures down to 15 mK in magnetic fields up to 7 Tesla on different intermetallic systems, which are located close to a quantum phase transition. Both heavy-fermion systems like $YbRh_2(Si_{1-x}Ge_x)_2$ and $CeAu_2In_4$ as well as transition metal oxides ($Sr_{1-x}Ca_xRuO_3$ thin films) are investigated. The results are compared with different theoretical scenarios. Our work is supported by the DFG through SFB 602 and research unit "Quantum phase transitions".

TT 27.25 Wed 14:00 Poster D1

Quantum Dissipation in Spin Systems: Spin-Boson Model and its Quantum Phase Transition — •André Winter and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, Campus, 66123 Saarbrücken

Our interest is focused on quantum-dissipative effects in spin systems. These effects play a highly interesting role in several fields of physics, like the decoherence of qubits or charge transfer in donor-acceptor systems. Mainly, the spin-boson model, which describes a two-level system coupled to a bosonic bath with a spectral density $J(\omega) \propto \omega^s$ will be discussed. We developed a new Monte Carlo algorithm to explore the quantum phase transition between the localized and delocalized phase of this model in the sub-Ohmic regime ($0 < s < 1$). The applied method, which is based on the path integral approach to Quantum Monte Carlo computations, works in continuous time and uses cluster updates of worldline-segments to investigate the quantum critical point effectively.

In addition, we are considering extensions within this framework like an alternative approach, where the bosonic environment is simulated explicitly or more general setups with multiple interacting spins.

[1] A. Winter, H. Rieger, M. Vojta, and R. Bulla, Phys. Rev. Lett. 102, 030601 (2009)

TT 27.26 Wed 14:00 Poster D1

Shubnikov-de Haas oscillations in $Ca_3Ru_2O_7$ under pressure — •Lina Klintberg[1], Swee Goh[1], Naoki Kikugawa[2,3], Andrew Mackenzie[2], Michael Sutherland[1], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CB3 0HE, United Kingdom — [2]School of Physics and Astronomy, University of St. Andrews, St. Andrews, Fife KY16 9SS, United Kingdom — [3]National Institute for Materials Science, 1-2-1 Sengen, Tsukuba 305-0047, Japan

The bilayer ruthenate $Ca_3Ru_2O_7$ undergoes a series of phase tran-

sitions on cooling, which lead to a low carrier density state at low temperature. Hydrostatic pressure is applied on this material in order to track the Fermi surface whilst tuning and ultimately suppressing the high temperature phase transitions. Quantum oscillations in the Hall component of $Ca_3Ru_2O_7$ are investigated as a function pressure using a piston-cylinder cell. As the pressure is increased, the oscillation frequency decreases systematically, suggesting that the Fermi pockets shrink. Owing to the size of the frequencies and to the non-linear background, the evolution of the effective masses cannot be determined accurately enough to extract a trend other than that they remain of the order of $0.6m_e$. Further work at higher pressures is under way, using anvil cells, to track the evolution of the Fermi surface through the pressures where the magnetic and structural transitions eventually are suppressed.

TT 27.27 Wed 14:00 Poster D1

Quantum phase transition in a two-subband quantum wire — •Tobias Meng[1], Mehul Dixit[2], Markus Garst[1], Julia Meyer[3,2], and Achim Rosch[1] — [1]Universität zu Köln — [2]Ohio State University — [3]Universite Joseph Fourier Grenoble

We consider a quantum wire with two subbands close to the Lifshitz transition, at which the second band starts to get filled as a function of an external gate voltage. This quantum phase transition is, generically, characterized by pronounced correlations as the electrons in the second subband are strongly interacting: the diverging density of states close to the band bottom leads to unitary two-particle scattering in the low-energy limit. This effectively generates nodes in the many-body wavefunction of electrons with different spin polarization, and, as a result, the electrons in the second band behave effectively as spinless fermions. We argue that, as a consequence, the interaction between the subbands is dominated by non-local contributions similar to the case of spin-polarized electrons [1,2]. We present an analysis of the leading instabilities at small densities of particles in the second band.

[1] J.S. Meyer, K.A. Matveev, and A.I. Larkin, Phys. Rev. Lett. 98, 126404 (2007)

[2] M. Sitte et al., Phys. Rev. Lett. 102, 176404 (2009)

TT 27.28 Wed 14:00 Poster D1

The ferromagnetic phase transition in $Sr_{1-x}Ca_xRuO_3$ thin films studied by noise spectroscopy — •Adham Amyan[1], Pintu Das[1], Jens Brandenburg[2], Jens Müller[1], Melanie Schneider[3], Vasily Moshnyaga[3], and Philipp Gegenwart[3] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, Frankfurt am Main, Germany. — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany. — [3]Physikalisches Institut, Georg-August Universität Göttingen, Göttingen, Germany.

Fluctuation (noise) spectroscopy is a powerful tool to investigate the intrinsic dynamics of charge carriers coupled to lattice vibrations and defects, or magnetic and electronic excitations. In principle, one can access the autocorrelation function describing the kinetics of the fluctuating carriers. We employ an *ac*-technique to study the excess $1/f$-type noise at different temperatures and magnetic fields for samples $Sr_{1-x}Ca_xRuO_3$ with various Ca concentrations x. In particular, in our low-frequency studies we are interested in the energy distribution of fluctuators causing the excess noise in the vicinity of the ferromagnetic transition in the energy range of 1 meV-1 eV. To this end, we use a phenomenological random fluctuation model and compare the noise data to complementary measurements of the Hall effect. Also, we are investigating the differences of the low-temperature dynamical properties as a function of Ca doping, in particular close to the ferromagnetic quantum phase transition, where $T_C \to 0$ for $x_c = 0.7$.

Work supported by the DFG through the Emmy Noether-program and SFB 602.

TT 27.29 Wed 14:00 Poster D1

Multiple phase transitions in YbPd — •Stefanie Grünheit, Jeevan S. Hirale, Yoshifumi Tokiwa, and Philipp Gegenwart — I. Physik. Institut, Georg-August Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

Cubic YbPd is an interesting strongly-correlated electron system, as previous ^{170}Yb-Mössbauer measurements have suggested two different Yb charge states at low temperatures; one magnetic and the other one nonmagnetic in equal proportions [1]. We have synthesized large YbPd polycrystals and investigate their physical properties by electrical resistivity, magnetic susceptibility, specific heat and thermal expansion at temperatures down to 20 mK. Four phase transitions at 0.6 K, 1.9 K, 105 K and 125 K are found. While the two higher ones are presumably related to a structural distortion, which may result in two inequivalent Yb-sites, the two lower ones are of clear antiferromagnetic origin. At lowest temperatures, the Sommerfeld coefficient amounts to 200 mJ/(mol K^2) and a reduced entropy of about one quarter of $R \log 2$ at 1.9 K is found. These results are discussed in terms of a coexistence of mixed-valent and magnetic Yb-sites. To investigate the microscopic origin of the various transitions, synchroton and neutron scattering experiments are under way.

Work supported by DFG through research unit 960 (Quantum phase transitions).

[1] P. Bonville et al., Phys. Rev. Lett. 57 (1986) 2733.

TT 27.30 Wed 14:00 Poster D1

Metal-insulator transitions in layered ruthenates — Johanna Brand[1], •Anna Silex[1], Olaf J. Schumann[1], Michael Gottschlich[1], Steven Price[1], Navid Qureshi[1], Paul Steffens[1,2], Daniel Löwen[1], Yvan Sidis[3], Arsène Goukassov[3], Beatrice Gillon[3], Satoru Nakatsuji[4], Jason Farrell[5], Naoki Kikugawa[5], Andrew Mackenzie[5], Karin Schmalzl[2], and Markus Braden[1] — [1]II. Physik, Uni Köln — [2]ILL, Grenoble — [3]LLB, Saclay — [4]ISSP, Tokio, Japan — [5]Univ. of St. Andrews, Scotland

Ca- and Sr-Ruthenates are far more interesting than the structural similarity with the cuprates initially suggested. By doping the single or double layer materials, many interesting phenomena are observed. Substituting Ti into Sr_2RuO_4 stabilizes a spin-density wave (SDW) phase that still is metallic, in which the static ordering corresponds to the dominating magnetic instability in pure Sr_2RuO_4. On the other hand, the doping of Ti into the double layer material $Sr_3Ru_2O_7$ seems to induce a SDW type magnetic order with larger impact on the electronic properties. The SDW phase in Ti-doped $Sr_3Ru_2O_7$ does not seem to be related with the magnetic instabilities of the parent phase. In both Sr-ruthenates the impact of the Ti-doping on the crystal structure is small and changes slightly across the magnetic transition. However, we find a strong influence of the Ti-substitution in Ti-doped $Ca_3Ru_2O_7$ which significantly stabilizes a weakly non-metallic phase. This can be seen in the transition temperature and in the resistivity jump. A pronounced flattening of the lattice is discussed as a general feature accompanying the metal-insulator transition in layered ruthenates.

TT 27.31 Wed 14:00 Poster D1

Doping dependent behaviour of potassium intercalated pentacene films: watching out for correlation effects — •Andreas Ruff[1], Joep Loos[1], Michael Sing[1], Jens Pflaum[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg — [2]Experimentelle Physik 6, Universität Würzburg

Recently, evidence for a band-filling controlled Mott metal-insulator transition (MIT) was reported for strongly potassium (K) doped pentacene (PEN) films on silicon substrates by conductivity measurements [1]. We have investigated the system K_xPEN on silicon with different orientations by means of photoelectron spectroscopy to follow the evolution of the spectral function with doping. The high quality of our PEN films is demonstrated by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED) measurements. In the ultraviolet photoemission spectra (UPS) one can observe the gradual filling of the former lowest unoccupied molecular orbital (LUMO) with K evaporation time. Additionally, conductivity measurements have been carried out to observe the MIT. To clarify the growth mode of the films images of the surface were taken with an atomic force microscope (AFM). Despite the drastic change in conductivity, no spectroscopical evidence neither for the metallic regime nor for the Mott transition has been observed as yet.

[1] M.F. Craciun et al, PRB 79, 125116 (2009)

TT 27.32 Wed 14:00 Poster D1

The metal-to-insulator transition in organic charge-transfer salts studied by noise spectroscopy — •Robert Rommel[1], Pintu Das[1], Adham Amyan[1], Jens Müller[1], Jens Brandenburg[2], and Dieter Schweitzer[3] — [1]Goethe-Universität Frankfurt, SFB/TR49, Frankfurt am Main — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden — [3]3. Physikalisches Institut, Universität Stuttgart

The organic $(ET)_2X$ compounds are model systems for low-dimensional metals exhibiting both strong electronic correlations and electron-phonon interactions. In particular, the interplay of onsite and intersite Coulomb interaction on the one hand and the coupling to the

lattice degrees of freedom on the other hand are interesting to investigate with respect to the different kinds of metal-to-insulator transition (MIT) in this class of materials. We employ a new technique, fluctuation (noise) spectroscopy, for the quasi-2D $(ET)_2X$ salts to study the low frequency dynamics of the correlated electrons. Our experimental setup allows for measuring the resistance fluctuations in the frequency range from 1 mHz to above 100 Hz for systems showing an MIT in a wide temperature range covering variations of the samples' resistance noise of many orders of magnitude (e.g. $10^{-8}-10^{6}\,\Omega^2/\mathrm{Hz}$). We employ a simple random fluctuation model to study the distribution of activation energies of the specific fluctuations causing the excess, 1/f-type noise. We compare different kinds of MIT regarding the mechanisms for slow electron dynamics.

TT 27.33 Wed 14:00 Poster D1

Pressure-induced phase transition in $ZnCr_2Se_4$ spinel — •Kaneez Rabia[1], Leonetta Baldassarre[1], Vladimir Tsurkan[2,3], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, Germany — [2]Experimentalphysik V, Universität Augsburg, Germany — [3]Insitute of Applied Physics, Academy of Sciences of Moldova, Chisinau, Republic of Moldova

Among the various transition metal chalcogenide spinels, the chromium spinels with the formula ACr_2X_4, with A=Zn,Cd or Hg, and X=O,S or Se, were most extensively investigated because of their unusual optical, electrical, and magnetic properties. The Cr^{3+} ions with the electron configuration $3d^3$ occupy the B sites with an octahedral environment. Under the action of the octahedral crystal field the Cr 3d levels split into a lower t_{2g} triplet, each orbital being singly occupied, and an excited eg doublet; the resulting bulk material is a Mott insulator with S=3/2. These compounds show a wide variety of magnetic properties ranging from those of a strongly frustrated antiferromagnet to a Heisenberg ferromagnet.

In the present study we studied the optical response of $ZnCr_2Se_4$ in refection mode as a function or pressure. Our results suggest the occurrence of a sluggish structural phase transition and the tendency of charge delocalization starting from 12 GPa. We will also discuss the pressure dependence of the high-energy electronic excitations, which are assigned to onsite crystalfield transitions.

TT 27.34 Wed 14:00 Poster D1

Magnetic and electronic properties in Chromates $R\mathbf{CrO_3}$ and the Vanadate $\mathbf{K_2V_8O_{16}}$ (Hollandite) — •A. C. Komarek[1,2], M. Isobe[3], T. Möller[1], M. Hoelzel[4,5], A. Senyshyn[4,5], D. Trots[6], M. T. Fernandez-Diaz[7], T. Hansen[7], M. Azuma[8], Y. Ueda[3], J. Hemberger[1], T. Unruh[5], J. R. Stewart[7,9], M. Grüninger[1], D. I. Khomskii[1], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany — [2]TU München, Physics Departement E21, D-85748 Garching, Germany — [3]Institute for Solid State Physics, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan — [4]Technische Universität Darmstadt, Material und Geowissenschaften, Petersenstrasse 23, D-64287 Darmstadt, Germany — [5]TU München, FRM-II, Lichtenbergstr. 1, D-85747 Garching, Germany — [6]Hasylab/DESY, Notkestr. 85, D-22607 Hamburg, Germany — [7]Institut Laue-Langevin, 38042 Grenoble, France — [8]Institute for Chemical Research, Kyoto University, Uji, Kyoto 611-0011, Japan — [9]ISIS facility, Rutherford Appleton Laboratories, STFC, Chilton, Didcot OX11 0DE, UK

$CaCrO_3$ is a $3d^2$ transition metal oxide with perovskite structure. Regarding the magnetism in such correlated electron systems, ferromagnetism usually comes along with metallic and antiferromagnetism (AFM) with insulating properties. Due to our neutron and optical measurements $CaCrO_3$ seems to be a rare example of a fully 3-dim. AFM transition metal oxide. $K_2V_8O_{16}$ is a mixed-valent vanadium oxide which exhibits a MI-transition at 160 K. Below T_{MI} we found a strong dimerization resembling on the monoclinic M2-phase in VO_2.

TT 27.35 Wed 14:00 Poster D1

Temperature dependent optical conductivity of $\mathbf{RVO_3}$ (R=Y, Gd), $\mathbf{LaSrFeO_4}$ and $\mathbf{RCoO_3}$ (R=La, Eu) studied by ellipsometry — •Julia Küppersbusch[1], Kostiantyn Shportko[1], Agung Nugroho[2], Thomas Palstra[2], Navid Qureshi[1], Marco Reuther[1], Thomas Lorenz[1], and Markus Grüninger[1] — [1]Universität zu Köln — [2]Rijksuniversiteit Groningen

Spin and orbital degrees of freedom play a decisive role in strongly correlated transition-metal oxides. Spin and orbital correlations for instance have a strong impact on the optical transitions from the lower to the upper Hubbard band. Our aim is a systematical study to understand the importance of spin/orbital correlations and also excitonic effects on the temperature dependence of the optical spectra. We use ellipsometry from 0.75 to 5.5 eV and show results on RVO_3, $LaSrFeO_4$, and $RCoO_3$.
The $3d^5$ configuration of $LaSrFeO_4$ does not show orbital degrees of freedom, the spins order at 350 K, thus the behavior at lower temperatures offers a reference for the influence of the lattice. The T dependence of the optical data of $3d^2$ RVO_3 can be well described on the basis of spin/orbital correlations. The $3d^6$ compounds $RCoO_3$ allow to study the effect of a spin-state transition on the optical data.

TT 27.36 Wed 14:00 Poster D1

LDA+DMFT study of $LaCoO_3$ — •Evgeny Gorelov and Eva Pavarini — IFF and IAS, Forschungszentrum Jülich, 52425 Jülich

$LaCoO_3$ has attracted a lot of attention because of its spin-state transitions, the nature of which has been debated since decades. In this work we study $LaCoO_3$ by means of the LDA+DMFT (local-density approximation + dynamical mean-field theory) method. Using the downfolding procedure based on the N-th Order Muffin-Tin Orbital approach, we calculate ab-initio $3d$ Wannier functions and construct the corresponding 5-band Hubbard model. We solve this model within dynamical mean-field approximation. We use the weak-coupling CT-quantum Monte Carlo method as impurity solver; this allows us to take into account the full rotationally-invariant Coulomb interaction, including the pair-hopping and spin-flip terms. We also retain the full self-energy matrix in orbital space. We analyze the competition between crystal-field splitting and Hund's rule coupling.

TT 27.37 Wed 14:00 Poster D1

Variational Monte Carlo study of the one-dimensional $t-t'$ Hubbard model — •Luca F. Tocchio[1], Claudius Gros[1], and Federico Becca[2] — [1]Institute for Theoretical Physics, Goethe-University Frankfurt, Max-von-Laue-Straße 1, D-60438 Frankfurt am Main, Germany — [2]CNR-INFM-Democritos National Simulation Centre and International School for Advanced Studies (SISSA), Via Beirut 2, I-34151 Trieste, Italy

We present a Variational Monte Carlo study of the one-dimensional Hubbard model with nearest and next-nearest neighbour hopping. After settling the metal-insulator transition, we describe the spin properties of the model, studying their behaviour across the metal-insulator transition and inside the insulating phase. The spin properties are then shown to be related to the single-particle spectrum in the optimized variational wave function. Moreover, we find that the metal-insulator transition can be already characterized at a mean-field level, since the underlying Fermi surface renormalizes to perfect nesting at the transition.

TT 27.38 Wed 14:00 Poster D1

Spectral properties of the three-dimensional Hubbard Model — •Sebastian Fuchs[1], Emanuel Gull[2], Matthias Troyer[3], Mark Jarrell[4], and Thomas Pruschke[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Department of Physics, Columbia University, W 120th Street New York, NY 10027, USA — [3]Institut für Theoretische Physik, ETH Zürich, Wolfgang-Pauli-Str. 27, 8093 Zürich, Switzerland — [4]Louisiana State Universtity, Baton Rouge, LA 70803, USA

We calculate momentum resolved single-particle spectra of the three-dimensional Hubbard Model. We perform Quantum Monte Carlo (QMC) simulations inside and outside the antiferromagnetically symmetry broken phase in the vicinity of the metal-insulator transition. The full lattice model is approximated by the Dynamical Cluster Approximation (DCA) and the resulting cluster model is solved using a QMC algorithm in continuous imaginary time. The absence of a time discretization error and Monte Carlo measurements in Matsubara frequencies enable us to analytically continue the self-energies directly by a Maximum Entropy calculation. Thus, momentum resolved single-particle spectra can be determined using Dyson's equation.

TT 27.39 Wed 14:00 Poster D1

The role of the double counting correction in the LDA+DMFT method - a systematic study. — •Michael Karolak, Tim Wehling, German Ulm, and Alexander Lichtenstein — I. Institut für theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg

An intrinsic issue of the LDA+DMFT approach is the so called double-

counting of interaction terms. How to choose the double-counting potential in a manner that is both physically sound and consistent is unknown. We have conducted an extensive study of the charge transfer system NiO in the LDA+DMFT framework using quantum Monte Carlo and exact diagonalization as impurity solvers. By explicitely treating the double-counting correction as an adjustable parameter we systematically investigated the effects of different choices for the double-counting on the spectral function. Different methods for fixing the double counting can drive the result from Mott insulating to almost metallic.

TT 27.40 Wed 14:00 Poster D1

Non-linear integral equations for transfer matrices of Chalker Coddington network models — •Win Nuding and Michael Brockmann — Bergische Universitä Wuppertal, Germany

We analyse the eigenvalues of the transfer matrices of an integrable Chalker Coddington model on the basis of the work by Gade and by Essler, Frahm and Saleur. We derive from the Bethe ansatz equations a finite system of non-linear integral equations. Whereas in the Bethe ansatz the system size L is equal to the number of unknown Bethe ansatz roots, L enters the non-linear integral equations just as an external control parameter. We present solutions of the non-linear integral equations. From these the eigenvalues of the transfer matrices are obtained.

TT 27.41 Wed 14:00 Poster D1

Calculating Thermodynamic Properties using Stochastic Sampling within the DMRG framework — •Stefan Kremer[1,2] and Peter Schmitteckert[3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Laboratoire CRISMAT, UMR 6508 CNRS-ENSICAEN, and IRMA, Caen, France — [3]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

In order to calculate thermodynamic properties a method within the framework of the Density Matrix Renormalisation Group (DMRG) is proposed. This method combines the Imaginary Time Evolution with the ideas of Stochastic State Sampling proposed by J. Jaklič and P. Prelovšek. In their approach obtaining thermodynamic states within Exact Diagonalisation is accomplished by the means of stochastic sampling of the Hilbert space. Thermodynamic expectation values of conserved quantities at a specific temperature can then be evaluated since they correspond to the quantum mechanical expectation values with respect to such states. Performing an evolution of the states in imaginary time will therefore represent a cooling of the system. In the proposed method the Hilbert space is sampled stochastically where the low energy region is sampled with a higher weight for the purpose of evaluating the thermodynamic expectation values at low temperature. Results for the specific heat of spinless fermionic rings are compared to predictions from Exact Diagonalisation.

TT 27.42 Wed 14:00 Poster D1

Screening of U in a three-band Hubbard model — •Clemens Adolphs and Erik Koch — German Research School for Simulation Sciences, FZ-Jülich and RWTH Aachen University, 52425 Jülich

We study the screening of the Hubbard interaction. As a concrete example, we consider a three-band Hubbard model with a central, half filled band, one filled band below, and an empty band above. We use the Lanczos algorithm to solve this model for small chains and calculate the spectral function. We then investigate a one-band Hubbard model where the renormalized interaction energy, U, for the one-band Hubbard model is calculated from the charging energy of the central orbital in the atomic limit of the original model. Comparing the spectral functions of the two models, we determine in which cases a one-band description using such a static renormalized U is feasible.

TT 27.43 Wed 14:00 Poster D1

Variational matrix product states for nano chains — •Andrej Schwabe and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany

We discuss a variational matrix product states (VMPS)[1,2] code, where the coefficients of the test wave function Ψ are assumed as product of site dependent matrices $\mathbf{A}^i$. The advantageous matrix product operator (MPO) representations is used, which allows to construct a generic algorithm, almost independent of the Hamiltonian H. In order to optimize the code and to account for physical properties of H, the wave function transformation as well as $U(1)$ symmetries have been implemented. Furthermore, the corrected one-site algorithm, recently proposed by White [3], is incorporated in our VMPS code at several approximation stages. We perform a benchmark test to study the impact of both the corrected one-site algorithm and the implementation of the $U(1)$ symmetries on CPU time and accuracy of the results.
The technique is applied to ferromagnetic nano chains in one dimension, described by inhomogeneous Hubbard-type models with site dependent Hubbard-U. The magnetic phase diagram and its dependence on the chain length are investigated. We discuss the emergence of the magnetic exchange coupling (e.g. RKKY) within and between the nano particles. Size and distance dependencies are studied as well as the competition with the Kondo effect.

[1] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005)
[2] F. Verstraete et al., Advances in Physics **57**, 143 (2008)
[3] S. R. White, Phys. Rev. B **72**, 180403 (2005)

TT 27.44 Wed 14:00 Poster D1

On the existence of the excitonic insulator phase in the extended Falicov-Kimball model: a vectorial slave-boson approach — •Bernd Zenker[1], Dieter Ihle[2], Franz Xaver Bronold[1], and Holger Fehske[1] — [1]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17489 Greifswald, Germany — [2]Institut für Theoretische Physik, Universität Leipzig, 04109 Leipzig, Germany

Motivated by the possibility of pressure-induced exciton condensation in intermediate-valence Tm[Se,Te] compounds we study the Falicov-Kimball model extended by a finite f-hole valence bandwidth. Within slave-boson mean-field theory we show that coherence between c- and f-states may be established at low temperatures, leading to an excitonic insulator (EI) phase. Thereby our vectorial slave-boson approach overcomes (i) the difficulties of the scalar slave-boson scheme by describing the EI state, and yields (ii) a substantial reduction of the critical temperatures in comparison to those of the standard Hartree-Fock approach. Analyzing the partial densities of states we find strong evidence that the EI typifies either a BCS condensate of electron-hole pairs (weak-coupling regime) or a Bose-Einstein condensate (BEC) of preformed excitons (strong-coupling regime), which points towards a BCS-BEC transition scenario as Coulomb correlations increase.

TT 27.45 Wed 14:00 Poster D1

Structural and Magnetic Properties of Fe Obtained by Dynamical Mean-Field Theory — •Ivan Leonov[1], Alexander I. Poteryaev[2], Vladimir I. Anisimov[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia

We present an application of a novel *ab initio* approach to calculate the total energy of materials with correlated electrons [1,2]. It combines band structure and dynamical mean-field theory, and is implemented in terms of plane-wave pseudopotentials. Here we employ this computational scheme to study structural and magnetic properties of elemental Fe at finite temperatures. For this purpose we analyzed the energetics of the *bcc-fcc* lattice transformation in Fe using the Bain transformation path. We find that at ambient pressure the temperature of the *bcc-fcc* structural phase transition occurs at ∼200 K above the calculated Curie temperature. The structural optimization performed for paramagnetic Fe yields the correct lattice constants and predicts a 2 % shrinking of the volume at the *bcc-fcc* phase transition.

[1] I. Leonov, N. Binggeli, Dm. Korotin, V. I. Anisimov, N. Stojić, and D. Vollhardt, Phys. Rev. Lett. **101**, 096405 (2008).
[2] I. Leonov, Dm. Korotin, N. Binggeli, V. I. Anisimov, and D. Vollhardt, arXiv:0909.1283 (2009).

TT 27.46 Wed 14:00 Poster D1

Modified Fermi-liquid behavior of the Hubbard model at finite temperature within the dynamical mean-field theory — •Sebastian Schmitt — Lehrstuhl für Theoretische Physik II, Technische Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund

The one-particle Green function of the Hubbard model is calculated within the dynamical mean field theory (DMFT) for various non-interacting density of states (DOS). The Fermi-liquid ground state usually observed within the DMFT reveals itself through the characteristic quadratic minimum in the imaginary part of the self-energy which develops already at finite temperature. In situations where the non-interacting DOS features van-Hove singularities in the vicinity of the Fermi level, this minimum at finite temperature is strongly modi-

fied and may even transform into a maximum. The presented findings are discussed in connection with non-Fermi liquid and pseudogap behavior usually encountered in non-local extensions of the DMFT.

TT 27.47 Wed 14:00 Poster D1

Projected excitations in a generalized Gutzwiller approximation — •Andrea Di Ciolo and Claudius Gros — Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, Frankfurt am Main, Germany.

We extended the generalized Gutzwiller Approximation originally proposed in PRB 72, 144505 (2005) to study projected particle (hole) excitations for inhomogeneous systems with SDW and/or CDW.

This method allows to evaluate observables associated to a correlated state with one or more excitations: for single excitations, one can evaluate their tunnelling transition probabilities into the correlated state; for double excitations one can investigate the response of the system... This approach is conceptually very powerful, because it allows a model-independent analysis: this means that the results are due only to the physical properties of the trial state and not to the choice of a specifical Hamiltonian. The drawback is that the complete extension of the formalism is very challenging, because new Gutwiller factors arise beyond the standard ones, obtained for example in Supercond. Sci. Tech. 1, 36, (1988). In particular, one task is highly not trivial: the evaluation of the size of the Hilbert spaces associated to a physical correlated state and to auxiliary ones. In order to learn how to handle the subtleties of the extended scheme, we applied it first to the case of the AFM. These latter results can be compared to the experimental evidence for materials displaying a long-range AFM order.

TT 27.48 Wed 14:00 Poster D1

Influence of Spin Fluctuation on the Single and Two Particle Properties of Two Dimensional Correlated System — •B.D Napitu[1,2] and J Berakdar[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik Heinrich-Damerow-Str.4 D-06120 Halle (Saale),Germany — [2]Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, D-06120 Halle, Germany

We inspect the interplay between spin fluctuations and the local Coulomb repulsion in strongly correlated two dimensional systems using the Hubbard model. By employing a state-of-the-art extended dynamical mean field theory (EDMFT) that incorporates the non-local interaction in the conventional single site dynamical mean field theory (DMFT), the single particle spectral function, the dynamical spin susceptibility and two particle quantities are calculated. It is shown that the inclusion of spin fluctuation assists the formation of pseudogap in the single particle spectral function. Similarly, the particle-particle sector also shows a reduction of the spectral weight as the spin exchange interaction increases.

TT 27.49 Wed 14:00 Poster D1

Perturbative theory of isosbestic points — •Markus Greger, Marcus Kollar, and Dieter Vollhardt — Theoretische Physik III, Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg

A family of non-monotonic curves, obtained by plotting a quantity $f(x, y)$ as a function of one of its variables (say, x) for different values of y, will in general intersect, leading to crossing points of the curves. In physics, chemistry and biology the crossing of a family of curves is the rule rather than the exception. Sometimes these crossing points are found to be confined to a remarkably narrow region, or are even located at a single point, thus leading to a conspicuous feature often called *isosbestic point*. Here we consider a perturbative expansion in the variable y. For an *exact* isosbestic point $x^\star$, the dependence of $f(x, y)$ on y is then described by the first term of the expansion in y. For *approximate* isosbestic points higher order terms are responsible for the finite width of the crossing region. This approach describes approximate isosbestic points in various unrelated quantities such as the optical conductivity $\sigma(\omega, n)$ in the Falicov-Kimball model, the photoemission spectra $A(\omega, T)$ of VO_2/TiO_2, the reflectivity $R(\omega, T)$ of $CaCu_3Ti_4O_{12}$, and the Raman response $\chi''(\omega, T)$ of $HgBa_2CuO_{4.16}$.

TT 27.50 Wed 14:00 Poster D1

Thermodynamic properties of the Hubbard model — •Patrick Haase[1], Sebastian Fuchs[1], Mark Jarrell[2], and Thomas Pruschke[1] — [1]Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37075 Göttingen, Germany — [2]Louisiana State Universtity, Baton Rouge, LA 70803, USA

We calculate the temperature dependence of the internal energy of the Hubbard model in the dynamical mean field approximation using continuous-time quantum Monte Carlo simulations. We fit the energy data with the density of states of a non-interacting system. With this density of states we are able to calculate thermodynamic properties like the entropy, which is not directly accessible by Monte Carlo simulations.

TT 27.51 Wed 14:00 Poster D1

High-frequency tails and the decay rate of high-energy excitations in correlated systems — •Matthias Sitte[1] and Lev Ioffe[2] — [1]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln — [2]Center for Materials Theory, Department of Physics and Astronomy, Rutgers University, Piscataway NJ 08854 USA

For energies much larger than the bandwidth, the lifetime of a highly excited state becomes exponentially large. Similarly, the high-frequency tails of correlation functions decay exponentially. This response is due to a collective excitation of many discrete degrees of freedom. Such a many-particle scattering process describes, e.g., the decay of doublons (doubly occupied sites) in ultra-cold atom gases in optical lattices, or the NMR relaxation mechanism in large magnetic fields. Here, we investigate the shape of correlation functions at high frequencies. In particular, we consider the spin 1/2 Heisenberg XXZ chain, a paradigm model for strongly correlated systems, which can be realized, e.g., in spin chain systems and in ultra-cold atom gases using two-level systems. Using exact diagonalization methods we calculate the correlation function of the staggered magnetization in frequency space and compare to analytical approaches.

TT 27.52 Wed 14:00 Poster D1

Eigenexcitation of Anderson impurity model out of equilibrium — •Pei Wang and Stefan Kehrein — Arnold Sommerfeld Center, department of physics, LMU

We solve the Anderson impurity model out of equilibrium by searching for the eigenexcitation operator A, which is defined as [H,A]=EA. We express the fermion creation and annihilation operators by eigenexcitation operator to calculate the time evolution. Then we transform back to calculate the expectation value. This method is compared to the flow equation method. It is better for considering the correction to eigen energy.

TT 27.53 Wed 14:00 Poster D1

Non-equilibrium steady state in a periodically driven Kondo model — Markus Heyl and •Stefan Kehrein — Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 München

We investigate the Kondo model with time-dependent couplings that are periodically switched on and off. On the Toulouse line we solve the problem exactly by using bosonization and refermionization that are also suitable for the Kondo model out of equilibrium [1]. We derive exact analytical results for the spin dynamics in the steady state that builds up after an infinite number of switching periods. Remarkably, the algebraic long time behavior of the spin-spin correlation function remains completely unaffected by the driving. In the limit of slow driving the dynamics becomes equivalent to that of a single interaction quench. In the limit of fast driving one can show that the steady state cannot be described by some effective equilibrium Hamiltonian since a naive implementation of the Trotter formula gives wrong results. As a consequence, the steady state in the limit of fast switching serves as an example for the emergence of new quantum states not accessible in equilibrium.

[1] D. Lobaskin and S. Kehrein, Phys. Rev. B **71**, 193303 (2005).

TT 27.54 Wed 14:00 Poster D1

spatiotemporal formation of the Kondo screening cloud — •Alexander Hoffmann and Stefan Kehrein — Physics Department, ASC, and CeNS, Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 Munich, Germany

The Kondo model is the paradigm for describing correlated quantum impuritites. Its equilibrium properties are well known, but its non-equilibrium behavior has recently attracted a lot of attention. We calculate the time dependent spin-spin correlation function between the impurity spin and the conduction band spin after a sudden switching on of the interaction. This amounts to studying the spatiotemporal formation of the Kondo screening cloud. To this end we bosonize the Kondo model and then refemionize it at the Toulouse point.

TT 27.55 Wed 14:00 Poster D1

Non-equilibrium magnetization dynamics of ferromagnetically coupled Kondo spins — •Andreas Hackl[1], Matthias Vojta[1], Stefan Kehrein[2], Walter Hofstetter[3], and David Roosen[3] — [1]Universität zu Köln — [2]Universität München (LMU) — [3]Universität Frankfurt

An analytical description of non-equilibrium phenomena in interacting quantum systems is rarely possible. Here we present one example where such a description can be achieved, namely the ferromagnetic Kondo model. In equilibrium, this model is tractable via perturbative renormalization-group techniques. We employ a recently developed extension of the flow-equation method to calculate the non-equilibrium decay of the local magnetization at zero temperature. The flow equations admit analytical solutions which become exact at short and long times, in the latter case revealing that the system always retains a memory of its initial state.

TT 27.56 Wed 14:00 Poster D1

Scaling approach to a time-dependent Kondo model: from adiabatic switching to an interaction quench — •Constantin Tomaras and Stefan Kehrein — LMU München, Department für Physik und Arnold-Sommerfeld-Center for Theoretical Physics, Theresienstraße 37, D-80333 München, Germany

The time-dependent quantum many-body problem has become of particular interest within the recent years [1]. Less is known about the transition from adiabatic turning on the interaction to an interaction quench in generic many-body systems. For the Hubbard model the quench physics were accessible with the help of flow equations [2], while the transition to an adiabatic switching procedure has been investigated by means of Keldysh perturbation theory [3]. Here we consider the isotropic ferromagnetic Kondo model, in which the interaction is switched on according to the time-dependent exchange couplings $J_{kk'}(t)$. Following [4,5], a convenient measure of the deviation of the impurity-spin z-component, from idealized adiabatic evolution is the ratio $\mu = \langle 0|S^z(t\to\infty) - S^z|0\rangle / \left(\langle\tilde{0}|S^z|\tilde{0}\rangle - \langle 0|S^z|0\rangle\right)$. $|\tilde{0}\rangle, |0\rangle$ are the ground states of the interacting and non-interacting system. Applying some generalized renormalization scheme, the ratio μ is shown to interpolate continuously between its quenched and adiabatic value.

[1] M. Greiner et al. *Nature*, 419 (2002)
[2] M. Moeckel and S. Kehrein, *PRL*, 100 (2008)
[3] M. Moeckel and S. Kehrein, arXiv.org:0911.0875 (2009)
[4] A. Hackl, S. Kehrein, M. Vojta, arXiv.org:0908.3647 (2009) [5] A. Hackl et al. *PRL*, 102 (2009)

TT 27.57 Wed 14:00 Poster D1

Real-time simulations of nonequilibrium transport in the single-impurity Anderson model — •Fabian Heidrich-Meisner[1], Adrian Feiguin[2], Luis Dias Da Silva[3,4], George Martins[5], Carlos Bussser[5], Enrique Anda[6], and Elbio Dagotto[3,4] — [1]LMU Munich, Germany — [2]University of Wyoming, USA — [3]ORNL, USA — [4]University of Tennessee, USA — [5]Oakland University, USA — [6]PUC Rio, Brazil

In this work, we consider the single-impurity Anderson model and use the adaptive time-dependent density matrix renormalization group (tDMRG) method to compute real-time currents out of equilibrium [1]. We first focus on the particle-hole symmetric point where Kondo correlations are the strongest and then extend the study of the nonequilibrium transport to the mixed-valence regime. As a main result, we present accurate data for the current-voltage characteristics of this model. As tDMRG is typically implemented with a real-space representation of the noninteracting leads, the Kondo regime, due to the emergent exponentially large Kondo screening length, is difficult to access. We therefore also apply tDMRG to Wilson leads [2], i.e., noninteracting leads with a logarithmic discretization as used in the numerical renormalization group method, and show that in the limit of small biases, perfect conductance can be obtained from tDMRG at much smaller Kondo temperatures than using a real-space representation of the leads.

[1] F. Heidrich-Meisner et al., Phys. Rev B 79, 235336 (2009)
[2] L.G.G.V. Dias da Silva et al., Phys. Rev. B 78 195317 (2008)

TT 27.58 Wed 14:00 Poster D1

Transport simulations in correlated one-dimensional systems — •Malcolm Einhellinger and Alex Cojuhovschi — Leibniz Universität Hannover, Germany

We develop a numerical approach for investigating transport properties in correlated low-dimensional solids and nanosystems. The time-evolving block decimation method is used to simulate the nonequilibrium dynamics in finite one-dimensional lattices. Stationary transport properties are then obtained by scaling the finite-system results. The method is illustrated with the conductance of correlated one-dimensional conductors (Luttinger liquids) such as the Hubbard model and the spinless fermion model. Comparisons with exact results confirm the validity of our approach.

TT 27.59 Wed 14:00 Poster D1

Quantum Dynamics of a spin-boson system close to a classical phase transition — •Lutz Bakemeier, Andreas Alvermann, and Holger Fehske — Institut für Physik, Universität Greifswald, Deutschland

The Rabi model of a spin 1/2 coupled to a harmonic oscillator features a classical phase transition in the limit of zero oscillator frequency. While no phase transition exists in the full quantum model, the existence of the classical transition leads to interesting dynamics in the 'adiabatic limit' of small oscillator frequency. We begin with the characterization of the groundstate. From a simple variational ansatz, which is in good quantitative agreement with exact data, we deduce the relevant effects at different ratios of spin and oscillator frequency. Only at large oscillator frequency the model properties are explained through simple renormalization of the spin dynamics. Based on the groundstate characterization we discuss the Rabi quantum dynamics, with particular emphasis on the signatures of the classical phase transition, e.g. a lock-in of spin and oscillator dynamics. Our contribution shows that the Rabi model is a kind of generic model for the physics of different time-scales. The relevance for general spin-boson models and the connection to a general concept of 'polaron' physics are discussed.

TT 27.60 Wed 14:00 Poster D1

Superperturbation solver for non-equilibrium — •Alexander Lieder, Sergej Brener, Alexander Chudnovskiy, Dmytro Grytskyy, Christoph Jung, and Alexander Lichtenstein — I. Institut für Theoretische Physik

We present a generalization of the recently developed Superperturbation solver for the Anderson impurity model for the non-equilibrium case. The idea is to solve a small reference system using exact diagonalization with its full time dependence on the Keldysh contour and to treat the neglected bath degrees of freedom perturbatively. The key point is to introduce new fermionic degrees of freedom via a Hubbard-Stratonovich transformation. In the space of these auxiliary fermions Wicks theorem is applicable and a perturbation theory with a renormalized interaction is possible.

TT 27.61 Wed 14:00 Poster D1

Strongly Correlated Steady-State Transport through a Quantum Dot — •Andreas Dirks[1], Philipp Werner[2], Mark Jarell[3], and Thomas Pruschke[1] — [1]Universität Göttingen, Institut für theoretische Physik — [2]ETH Zürich, Institut für theoretische Physik — [3]Louisiana State University, Baton Rouge/LA, USA

We investigate the application of continuous-time Quantum Monte Carlo algorithms to the imaginary-time formalism introduced by Han and Heary [1]. The analytic structure of the two-variable Green's functions is discussed, and an algorithm for the numerical analytic continuation is proposed.

[1] J. E. Han, and R. J. Heary, Phys. Rev. Lett. **99**, 236808 (2007)

TT 27.62 Wed 14:00 Poster D1

Matrix product state approach for a two-lead, multi-level Anderson model — •Andreas Holzner, Andreas Weichselbaum, and Jan von Delft — Lehrstuhl für Theoretische Festkörperphysik, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany

We exploit the common mathematical structure of the numerical renormalization group and the density matrix renormalization group, namely matrix product states, to implement an efficient numerical treatment of a two-lead, multi-level Anderson impurity model. By adopting a star-like geometry, where each species (spin and lead) of conduction electrons is described by its own Wilson chain, instead of using a single Wilson chain for all species together, we achieve a very significant reduction in the numerical resources required to obtain reliable results, as illustrated for the occupation for a spinfull two-lead 4-level Anderson model. Moreover, we show that it is possible to find a

new "optimal" lead basis, obtained via a unitary transformation of the type $c_{\alpha k\sigma} \to U_{\alpha\beta}c_{\beta k\sigma}$ (where α and β label distinct leads), in which lead degrees of freedom on *different* Wilson chains are effectively decoupled from each other for all but the first few sites of each chain. This new basis turns out to also diagonalize the scattering matrix for the leads. We demonstrate this for a spinless two-lead, 4-level Anderson model, presenting DMRG-results for the mutual information between two sites located far apart on different Wilson chains, and NRG results for the scattering matrix.

TT 27.63 Wed 14:00 Poster D1

Coupled qubits in a dissipative environment — •Etienne Gärtner and Ralf Bulla — Institute of Theoretical Physics, University of Cologne, Germany

In recent years Numerical Renormalization Group (NRG) methods have not only been applied to systems of pure fermionic degrees of freedom. The successful application of NRG-techniques to the spin boson model has led to important insights on several technicalities one has to handle e.g. when dealing with a bosonic Hilbertspace and its unavoidable truncation. In the present case we study a system of two coupled qubits interacting with a dissipative environment. The dissipation is mediated through a bath of harmonic oscillators, thus we use a two-spin boson model to describe the system. In case of ohmic damping we calculate the entropy in a wide range of the parameter space to extract information about the ground state and the phase diagram.

TT 27.64 Wed 14:00 Poster D1

Exact diagonalization studies of small spin clusters Kondo-coupled to one-dimensional tight-binding electrons — •Martin Höck and Jürgen Schnack — Universität Bielefeld, Fakultät für Physik, D-33615 Bielefeld, Germany

Magnetic molecules are envisioned to store a single bit of information in future high-density information storage devices. For such an application it is necessary to graft the molecules on a substrate so that they can be individually addressed.

Motivated by the question of how the magnetic properties of a molecule are affected by the deposition on a surface, we study Kondo-Heisenberg model systems in which simple structures of exchange-coupled spins are interacting with one-dimensional tight-binding electrons. In particular, we focus on the magnetization of the spin cluster and examine, for different geometries, its dependence on an external magnetic field at finite temperatures. The effect of additional interaction terms like a single-ion anisotropy is also investigated.

In order to calculate the relevant thermodynamic observables, we perform a numerically exact, complete diagonalization of the model Hamiltonian. As the application of this method is limited to rather small systems, it is important to analyze the influence of finite-size effects. We investigate down to which temperatures reliable results, that adequately reflect the thermodynamic limit, can be obtained and how results for finite systems can be improved by e.g. boundary condition averaging.

TT 27.65 Wed 14:00 Poster D1

Thermal expansion and magnetostriction of the spin-$\frac{1}{2}$-chain compound $Cu(C_4H_4N_2)(NO_3)_2$ — •Jens Rohrkamp[1], Yvonne Sanders[1], Markus Garst[2], Matt D. Phillips[3], Mark M. Turnbull[3], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für theoretische Physik, Universität zu Köln, Germany — [3]Carlson School of Chemistry and Biochemistry, Clark University, USA

Compounds with magnetic subsystems representing simple model spin systems with weak magnetic coupling constants are ideal candidates to test theoretical predictions for the generic behavior close to quantum phase transitions. We present measurements of the thermal expansion and magnetostriction of the spin-$\frac{1}{2}$-chain compound copper pyrazine dinitrate $Cu(C_4H_4N_2)(NO_3)_2$. Of particular interest is the low-temperature thermal expansion close to the saturation field $H_c \approx 14\,\mathrm{T}$, which defines a quantum phase transition from the gapless Luttinger liquid state to the fully saturated state with a finite excitation gap. We find a sign change of the thermal expansion for the different ground states, and at the quantum critical point H_c the low-temperature expansion approaches a $1/\sqrt{T}$ divergence. Furthermore the magnetostriction data is compared to the spin-spin correlation function calculated via Bethe-Ansatz. This work was supported by the DFG through SFB 608.

TT 27.66 Wed 14:00 Poster D1

Magnetic Properties of the quasi-2D S=1/2 Heisenberg antiferromagnet $[Cu(pyz)_2(HF_2)]PF_6$ — •M. Ozerov[1], E. Čižmár[1,2], S.A. Zvyagin[1], R. Beyer[1], M. Uhlarz[1], Y. Skourski[1], J.L. Manson[3], J.A. Schlueter[4], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden, FZ Dresden - Rossendorf, Dresden, Germany — [2]Centre of Low Temperature Physics, P.J. Šafarik University, Košice, Slovakia — [3]Department of Chemistry and Biochemistry, Eastern Washington University, Cheney, WA, USA — [4]Materials Science Division, Argonne National Laboratory, Argonne, IL, USA

We report on ESR, magnetization, and specific-heat studies of $[Cu(pyz)_2(HF_2)]PF_6$ single crystals, identified as a quasi-two-dimensional spin-1/2 Heisenberg antiferromagnet. Our measurements revealed $J_{inter}/J_{intra} \leq 0.063$ and $A/J \sim 0.003$, where J_{inter}, J_{intra}, J are the interplane, intraplane and mean exchange interactions, respectively, and A is the anisotropy constant. It is argued that the magnetic properties of this material are strongly affected by two-dimensional spin fluctuations, despite of the onset of 3D long-range magnetic ordering at $T_N \approx 4.4$ K. The temperature-field phase diagram and ESR magnetic excitation spectrum in the 3D ordered phase of $[Cu(pyz)_2(HF_2)]PF_6$ will be discussed in detail.

This work was partly supported by the DFG and EuroMagNET (EU contract No. 228043)

TT 27.67 Wed 14:00 Poster D1

ESR Studies of the Quantum Spin Dimer System $Ba_3Cr_2O_8$ — •D. Kamenskyi[1], J. Wosnitza[1], S.A. Zvyagin[1], J. Krzystek[2], A.A. Aczel[3], H.A. Dabkowska[3], and G.M. Luke[3] — [1]Hochfeld-Magnetlabor Dresden, FZ Dresden - Rossendorf, Dresden, Germany — [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, USA — [3]McMaster University, Hamilton, Ontario, Canada

$Ba_3Cr_2O_8$ is a system of three-dimensionally coupled dimers, exhibiting a field-induced phase transition from a quantum-disordered to a long-range antiferromagnetically ordered state at $H_{c1} = 12.5$ T. We report tunable-frequency electron spin resonance (ESR) studies of $Ba_3Cr_2O_8$ single crystals performed in a frequency range between 50 and 700 GHz in fields up to 25 T (applied along the c axis). Two gaps in the magnetic excitation spectrum, $\Delta_1 = 564$ GHz and $\Delta_2 = 400$ GHz, were observed directly, confirming the spin-singlet ground state of $Ba_3Cr_2O_8$ below H_{c1}. The observation of singlet-triplet ESR transitions, which are normally forbidden in spin-1/2 dimer systems by selection rules, indicates the break-down of the axial symmetry in this compound. Details of the ESR excitation spectrum of $Ba_3Cr_2O_8$ across different regions of its phase diagram will be discussed.

This work was partly supported by the DFG and EuroMagNET (EU contract No. 228043).

TT 27.68 Wed 14:00 Poster D1

Magnetic properties of epitaxially strained $Sr_{1-x}Ca_xRuO_3$ thin films — •Markus Wissinger, Dirk Fuchs, and Hilbert v. Löhneysen — Institut für Festkörperphysik, Karlsruhe Institute of Technology, Karlsruhe, Germany

The magnetic properties of epitaxially strained $Sr_{1-x}Ca_xRuO_3$ thin films were investigated with respect to lattice changes caused by i) chemical pressure due to the substitution by smaller Ca ions as well as by ii) epitaxial strain due to the growth on different lattice matched substrate materials.

Stoichiometric polycrystalline targets were produced via standard solid state reaction for $0 \leq x \leq 1$. Thin epitaxial films were deposited from the targets by pulsed laser deposition on various substrate materials. The structural and magnetic properties of the bulk and thin film samples were characterized by x-ray diffraction and superconducting quantum interference device magnetometry.

The lattice parameters a, b, and c of the bulk as well as the out-of-plane lattice parameter of the thin film samples were found to decrease with increasing Ca substitution. The Curie temperature T_c also decreases with increasing x. Tensile or compressive strain in epitaxial films results in a significant increase or decrease of T_c , respectively, in comparison to the bulk value. The critical concentration, x_c, where $T_c = 0$ therefore shifts to higher or lower concentrations with respect to the bulk where x_c amounts to 0.7. The sensitivity of T_c to chemical pressure and epitaxial strain will be compared and discussed in detail.

TT 27.69 Wed 14:00 Poster D1

Spinon localization in the heat transport of the spin-1/2 ladder compound $(C_5H_{12}N)_2CuBr_4$ — •Gerhard Kolland[1], Jens

Rohrkamp[1], Beni Thielemann[2], Henrik M. Ronnow[3], Christian Rüegg[4], Karl Krämer[5], John A. Mydosh[1], Alexandr V. Sologubenko[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Lab. for Neutron Scattering, ETH Zürich & PSI Villigen, Switzerland — [3]Lab. for Quantum Magnetism, EPFL, Switzerland — [4]London Centre for Nanotech. and Dep. of Phys. and Astron., University College London, UK — [5]Dep. of Chem. and Biochem., University of Bern, Switzerland

Piperidium copper bromide $(C_5H_{12}N)_2CuBr_4$ is a two-leg spin-1/2 ladder system with comparatively weak antiferromagnetic exchange couplings along the legs and the rungs. Hence, this system has two experimentally accessible quantum phase transitions; from a gapped spin-singlet state to a gappless Luttinger-liquid state at $H_{c1} \simeq 7\,\mathrm{T}$ and from this state to a fully polarized state at $H_{c2} \simeq 14\,\mathrm{T}$. Here, we present experiments on the magnetic field-dependent thermal transport. The thermal conductivity is only weakly affected by the field-induced transitions at $H_{c1/c2}$, suggesting the absence of a direct contribution of the spin excitations to the heat transport. We observe, however, that the thermal conductivity is suppressed by the magnetic field deeply within the Luttinger-liquid state. These surprising observations are discussed in terms of localization of spinons within finite ladder segments and spinon-phonon umklapp scattering of the predominantly phononic heat transport. *Supported by the DFG through SFB 608.*

TT 27.70 Wed 14:00 Poster D1

Generalized t-J models derived systematically from Hubbard models in the doped case — •Simone A. Hamerla and Götz S. Uhrig — Technische Universität Dortmund,Lehrstuhl für Theoretische Physik I, 44221 Dortmund, Germany

Fermionic Hubbard models are mapped to generalized t-J models by a systematic change of basis using self-similar continous unitary transformations (s-CUTs) [1].
In the new basis, charge fluctuations affecting the number of double occupancies are eliminated. The mapping relies on the energetic separation of sectors with different numbers of double occupancies. Thus this energy separation is calculated using the Liouville formalism. In this way we obtain the range of validity of the mapping for the first time in dependence of the doping.
Three different s-CUTs are investigated for various truncation schemes on linear chains and square lattices.

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

TT 27.71 Wed 14:00 Poster D1

Field-induced effects near the mysterious low-temperature phase transition in the proposed spin-liquid system κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ — •Rudra Sekhar Manna[1], Mariano de Souza[1], Andreas Brühl[1], John A. Schlueter[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, SFB/TR 49, D-60438, Frankfurt (M), Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA

The charge-transfer salt κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$, a Mott insulator with a 2D triangular lattice structure, is considered as a likely candidate for a quantum-spin liquid. We have studied this material by measuring the uniaxial expansion coefficients α_i, the specific heat and magnetic susceptibility. The main observations are: (i) a pronounced in-plane (bc) anisotropy in α_i, implying significant T-dependent lattice distortions, and (ii) a pronounced phase-transition anomaly at 6 K. By employing a Grüneisen-scaling Ansatz, we have been able to separate the corresponding contribution to the specific heat. The entropy release suggests that the spin degrees of freedom alone cannot account for the phase transition [1]. While the 6 K transition is insensitive to the application of a magnetic field up to 10 T, the highest field accessible, distinct field dependencies have been found which set in at somewhat higher temperatures for magnetic fields along the b-axis of one particular high-quality crystal. Based on measurements as a function of temperature at constant field and isothermal field sweeps, an anomaly diagram was able to be constructed.

[1] R. S. Manna *et al.*, arXiv:0909.0718 (2009).

TT 27.72 Wed 14:00 Poster D1

Structural and magnetic properties of the mixed quantum antiferromagnet $Cs_2CuCl_{4-x}Br_x$ — •P. T. Cong, S. Belz, N. Krüger, F. Ritter, W. Assmus, B. Wolf, and M. Lang — Physikalisches Institut, Goethe-Universität, SFB/TR 49, D-60438 Frankfurt(M).

The two compounds, Cs_2CuCl_4 and Cs_2CuBr_4, have been classified as quasi-two-dimensional quantum antiferromagnets. Cs_2CuCl_4 shows long-range magnetic order, which can be described as a Bose-Einstein condensation of magnons, i.e., delocalized triplet excitations, whereas the iso-structural compound Cs_2CuBr_4, exhibits plateaus in the magnetization, indicating the localization of triplets. Here we present a systematic study of the magnetic properties in the $Cs_2CuCl_{4-x}Br_x$ ($0 \leq x \leq 4$) mixed system. All crystals were synthesized by a solution-growth method. Two structural variants - an A-type orthorhombic and a B-type tetragonal - were detected in this system depending on the growth conditions. A detailed structural phase diagram has been constructed, based on X-ray Rietveld refinement, SEM and thermal analysis. χ(T) measurements of crystals near the end members of the series reveal a broad maximum at T_{max} indicative of quasi-2D short range correlations. While for the Cl^-rich system $0 \leq x \leq 0.8$, T_{max} slightly increases with increasing Br^-, a much stronger increase of T_{max}.is observed for the Br-rich system for $2.8 \leq x \leq 4.0$.

TT 27.73 Wed 14:00 Poster D1

Magnetic properties of the new low-dimensional spin magnet α-$Cu_2As_2O_7$ — •Yulieth Arango[1], Evgenia Vavilova[2], Olga Volkova[3], Mahmoud Abdel-Hafez[1], Matthias Weil[4], Alexander Vasiliev[3], Vladislav Kataev[1], Rüdiger Klingeler[1], and Bernd Büchner[1] — [1]Leibniz-Institut für Festkörper und Werkstoffforschung IFW Dresden, Dresden, Germany — [2]Zavoisky Physical-Technical Institute of RAS, Kazan, Russia — [3]Physics Faculty, Moscow State University, Moscow, Russia — [4]Institute for Chemical Technology and Analytics, Vienna University of Technology, Vienna, Austria

The crystal structure of α-$Cu_2As_2O_7$ consists of two-dimensional infinite sheets (ab-plane) of [CuO_5] polyhedra stacked along the c-axis. The Cu^{2+} ($3d^5$, S=1/2) ions are connected via oxygen ligands in the Cu-O chains along the diagonal of the ab-plane. In this work we study the interplay between the crystal structure and magnetism of α-$Cu_2As_2O_7$ single crystals by measuring magnetic susceptibility, specific heat, high field electron spin resonance (HF-ESR), and nuclear magnetic resonance (NMR). The data reveal that in the spin sector Cu-O chains represent a realization of a quasi-one dimensional (1D) spin-1/2 anisotropic Heisenberg antiferromagnet with the nearest neighbor exchange constant $J \sim 160$ K. Due to residual 3D interactions α-$Cu_2As_2O_7$ orders antiferromagnetically at $T_N \simeq 11$ K. Below T_N two phases are identified: a collinear phase and a field B induced spin-flop phase at $B > B_C \simeq 1.8$ T.

TT 27.74 Wed 14:00 Poster D1

Electron spin resonance spectroscopy of a novel Ni based hybrid $S = 1$ chain — •F. Lipps[1], A. H. Arkenbout[2], A. Meetsma[2], T. T. M. Palstra[2], P. H. M. van Loosdrecht[2], V. Kataev[1], and B. Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, Dresden, Germany — [2]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

We present results of a multifrequency ESR and static magnetization study of single crystals of a new hybrid material that comprises arrays of one dimensional (1D) chains of $NiCl_6$ octahedra separated by a framework of organic molecules. The $Ni^{2+}(3d^8)$ ions in the $NiCl_6$ chain possess an integer spin $S = 1$. Thus, in case of the antiferromagnetic (AFM) coupling, such a chain may provide an experimental realization of a prominent 1D $S = 1$ Heisenberg model, the Haldane chain. In contrast to the $S = 1/2$ chain it has a nonmagnetic ground state and a gapped spectrum of spin excitations. The ESR response of the studied samples is characterized by a single well-defined lorentzian line with a g-factor of $g \simeq 2.2$. The T-dependence of the ESR intensity which is proportional to the static spin susceptibility as well as the bulk static magnetization reveal a low temperature maximum suggesting an AFM coupling of the order of ~ 24 K. In this low temperature regime the ESR signal broadens substantially which indicates a growth of the low-frequency AFM dynamic spin correlations. Remarkably, no indications of the development of the static local internal fields due to the long-range order are observed in the ESR spectra. We discuss a possible ground state and spin dynamics of the studied compound.

TT 27.75 Wed 14:00 Poster D1

Hole induced spin polarons in $LaCoO_3$ — •A. Alfonsov[1], E. Vavilova[1,2], V. Kataev[1], A. Podlesnyak[3], D.I. Khomskii[4], and B. Büchner[1] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical Technical Institute, RAS, 420029 Kazan, Russia — [3]Oak Ridge National Laboratory, P.O. BOX 2008 MS6494 Oak Ridge

TN 37831-6494, USA — [4]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

We report a comparative high field electron spin- (ESR), nuclear magnetic resonance (NMR) and static magnetization study of lightly hole-doped samples of $La_{0.998}Sr_{0.002}CoO_3$ and $La_{0.998}Ca_{0.002}CoO_3$. We have shown before [1] that small Sr doping of $LaCoO_3$ yields the spin-state polaron with a big spin value and large spin orbital coupling. The Ca^{2+} ion, in contrast to the Sr^{2+} ion, has almost the same ionic radii as the La^{3+} ion. Therefore, the substitution of Ca for La provides mainly a hole to the system without creating a sizeable crystal field distortion around the substituted Ca ion. This difference enables us to ascertain the roles of the introduced hole and the created crystal field distortion in the formation of the spin polarons. The data obtained on Ca and Sr doped $LaCoO_3$ samples provide experimental evidence that the introduced hole indeed plays the main role. We discuss a model of the formation of big spin polarons in $LaCoO_3$ due to a very small hole doping.

[1] A. Podlesnyak et al., Phys. Rev. Lett. 101, 247603 (2008)

TT 27.76 Wed 14:00 Poster D1

Magnetic anisotropy in the quasi one-dimensional Ising spin-1/2 chain system $BaCo_2V_2O_8$ — •Sandra Niesen, Gerhard Kolland, Martin Valldor, Oliver Heyer, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

$BaCo_2V_2O_8$ contains screw chains of CoO_6 octahedra which are running along the c axis of the tetragonal crystal structure and are separated by nonmagnetic Ba^{2+} und V^{5+} ions in the aa plane. Due to a compression of the octahedra along c the threefold degeneracy of the t_{2g} orbitals is lifted and the magnetic ground state can be described by an effective Ising spin-1/2 antiferromagnetic chain. Due to a finite inter-chain coupling, $BaCo_2V_2O_8$ shows long-range antiferromagnetic order below $T_N \simeq 5.5$ K with the spins oriented along c.
We have prepared single crystals of $BaCo_2V_2O_8$ by a spontaneous nucleation method. Here, we present measurements of the magnetization, the specific heat, the thermal expansion, magnetostriction, and the thermal conductivity in magnetic fields up to 17 T. Depending on the field direction, the magnetic field influence is highly anisotropic. In case of H parallel c, the Néel order is strongly suppressed already for low fields, and changes into an incommensurate phase above about 4 T. For fields perpendicular to c, the field influence is much weaker. Besides, this expected Ising anisotropy, we have discovered a new magnetic anisotropy for fields applied within the aa plane. For magnetic fields applied along [110] T_N is only weakly suppressed, while for fields applied along [100] T_N is completely suppressed for fields above about 10 T. *This work is supported by the DFG through SFB 608.*

TT 27.77 Wed 14:00 Poster D1

Derivation of the effective microscopic models for the frustrated antiferromagnets Cs_2CuCl_4 and Cs_2CuBr_4 from first principles — •Kateryna Foyevtsova, Ingo Opahle, Harald Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

The frustrated antiferromagnets Cs_2CuCl_4 and Cs_2CuBr_4 have been attracting a lot of attention as low-dimensional quantum systems with a variety of unconventional properties, such as, for instance, the spin-liquid state in Cs_2CuCl_4 or magnetization plateaux in Cs_2CuBr_4.

In order to provide a theoretical insight to the on-going discussion of the Cs_2CuCl_4 and Cs_2CuBr_4 effective models, we perform a comprehensive Density Functional Theory (DFT) study of the electronic properties of Cs_2CuCl_4 and Cs_2CuBr_4 and derive the tight-binding (TB) and Heisenberg models' parameters for the two compounds. We find that in Cs_2CuCl_4 electronic correlations play an important role for the correct description of the crystal structure and discuss the implications of such results for DFT calculations with commonly-used approximations for the exchange-correlation functional.

TT 27.78 Wed 14:00 Poster D1

DMRG Study of Anisotropic Triangular Heisenberg Lattice — •Andreas Weichselbaum[1] and Steven R. White[2] — [1]Ludwig-Maximilians-Universität, 80333 München — [2]University of California, Irvine, CA 92697, USA

The anisotropic antiferromagnetic two-dimensional triangular Heisenberg lattice for spin 1/2 describes certain classes of transition-metal oxides (TMOs) and chalcogenides (TMCs), clearly supported by experimental data. The understanding of the ground state properties of this kind of system from a theoretical point of view, however, has remained an extraordinary challenge. In the model under consideration, quasi-one-dimensional Heisenberg chains of uniform intrachain coupling strength J interact with their neighboring chains via the interchain coupling J0. By varying the anisotropy ratio $j \equiv J'/J$ from $j = 0$ (decoupled Heisenberg chains) to $j = 1$ (uniform triangular lattice with finite Neel order like local magnetization), it was pointed out in previous studies [1] that, indeed, there appears to exist spin liquid properties up to remarkably high values of j of about 0.85. We given an update on our DMRG studies specifically optimized to reduce finite size effects [2].

[1] S. Yunoki et al., PRB 74, 014408 (2006).
[2] S. R. White et al., PRL 99, 127004 (2007).

TT 27.79 Wed 14:00 Poster D1

DMRG calculations for S=1 anisotropic Heisenberg antiferromagnetic chains — •David Peters[1], Ian P. McCulloch[2], and Walter Selke[1] — [1]JARA-SIM and RWTH Aachen, Institut für Theoretische Physik, Germany — [2]University of Queensland, Department of Physics, Brisbane, Australia

Using density matrix renormalization group calculations, for finite number of sites and in the thermodynamic limit, ground state properties of spin–1 Heisenberg chains with exchange and quadratic single-ion anisotropies in an external field are studied, for special choices of the two kinds of anisotropies [1,2]. In particular, the phase diagram includes antiferromagnetic, spin-liquid (or spin-flop), half magnetization plateau, and supersolid (or biconical) phases. Especially, generic features of the spin-liquid and supersolid phases as well as corresponding quantum phase transitions are discussed. Properties of the quantum chains are compared to those of corresponding classical spin chains.

Parts of the research has been funded by the excellence initiative of the German federal and state governments.

[1] D. Peters, I. P. McCulloch, W. Selke, Phys. Rev. B79, 132406 (2009); Journal of Physics: Conference Proceedings (in print)
[2] F. Heidrich-Meisner, I. P. McCulloch, A. K. Kolezhuk, Phys. Rev. B80, 144417 (2009)

TT 27.80 Wed 14:00 Poster D1

Dynamics of magnetic impurities in two-dimensional spin-1/2 antiferromagnets — •Björn Willenberg and Wolfram Brenig — Institut für Theoretische Physik, Technische Universität Braunschweig

Using Quantum Monte-Carlo methods based on the stochastic series expansion we investigate the dynamics of a single spin-1/2-degree of freedom coupled to a two-dimensional Heisenberg antiferromagnet (HAFM). Calculating imaginary time spin correlation functions and performing Maximum Entropy analysis we analyze the dynamical longitudinal and transverse local susceptibilities of the impurity. These quantities will be studied as a function of temperature and system size. Our findings will be compared to analytical results from stochastic Liouville equations. Finally we discuss the role of antiferro- versus ferromagnetic coupling of the impurity to the HAFM.

TT 27.81 Wed 14:00 Poster D1

Vacancies in non-collinear antiferromagnets — •Alexander Wollny, Lars Fritz, and Matthias Vojta — Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany

2D quantum Heisenberg antiferromagnets provide a variety of interesting phenomena. The role of vacancies has been widely studied on the square lattice, e.g. in the context of cuprates, and is reasonably well understood.

For a system with geometrical frustration the situation is more difficult. Here a magnetically ordered state often displays non-collinear order which has a strong influence on the basic excitations of the system, the spin-waves. The simplest realization is the triangular lattice which shows a 120° spin structure. At the classical level, a vacancy induces a local distortion of the spin pattern which partially relieves the frustration.

We perform a classical Monte Carlo simulation which determines the structure of the distortion and shows that it declines exponentially. Thus, it does not correspond to a goldstone mode but can be interpreted as a local condensate of spin-waves. Taken this distortion into account, we study the spin-wave corrections to the classical ground state in linear order and discuss how the vacancy could be seen in a local susceptibility measurement.

TT 27.82 Wed 14:00 Poster D1

Manipulating magnetic structures in chiral metals by cur-

rents — •Karin Everschor[1], Markus Garst[1,2], Rembert Duine[3], and Achim Rosch[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str.77, 50739 Köln — [2]Physik Department T30c, Technische Universität München, 85747 Garching — [3]Institute for Theoretical Physics, Department of Physics and Astronomy Faculteit Betawetenschappen, Utrecht University, Leuvelaan 4, 3584 CE Utrecht, The Netherlands

A Skyrmion is a topologically stable field configuration, originally introduced by Tony Skyrme, a nuclear physicist, who interpreted a proton as a "knot" in pion fields. Recently, the two-dimensional version of such Skyrmions was visualized as a lattice of vortices in the magnetic structure of manganese silicide (MnSi) We investigate theoretically the interaction between the applied electrical currrents and the topological magnetic structure.

TT 27.83 Wed 14:00 Poster D1

Ground state phases of the spin-1/2 J_1–J_2–J_3 Heisenberg antiferromagnet on the square lattice — •Rachid Darradi[1], Johannes Reuther[2], Wolfram Brenig[3], Johannes Richter[4], and Peter Wölfle[5] — [1]Institute for Theoretical Physics Technical University Braunschweig Mendelssohnstr. 3 38106 Braunschweig Germany — [2]Institute for Condensed Matter Theory University Karlsruhe, Postfach 6980 76128 Karlsruhe Germany — [3]Institute for Theoretical Physics Technical University Braunschweig Mendelssohnstr. 3 38106 Braunschweig Germany — [4]Institute for Theoretical Physics, Otto-von-Guericke University Magdeburg, 39016 Magdeburg, Germany — [5]Institute for Condensed Matter Theory University Karlsruhe, Postfach 6980 76128 Karlsruhe Germany

We investigate the zero-temperature phase diagram of the spin-1/2 frustrated J_1–J_2–J_3 Heisenberg Antiferromagnet on the square lattice. Using high orders coupled cluster method (CCM), Series expansion based on the flow equation method, and functional renormalization group (FRG), we have calculated the ground state energy, triplet excitations, the magnetic order parameter, and generalized susceptibilities. We determine the quantum critical lines for the semiclassical Néel, spiral and collinear phase, comparing our complementary approaches and contrasting our findings to other published results. Based on the susceptibilities which are related to valence-bond crystal order parameters we also discuss the nature of the quantum disordered phase separating the two semiclassical Néel and spiral phases.

TT 27.84 Wed 14:00 Poster D1

Consistent description of magnetic excitations and phase diagram of high-T_c cuprates within a strong-coupling approach — Sascha Brehm[1], •Enrico Arrigoni[2], Markus Aichhorn[3], and Werner Hanke[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute of Theoretical Physics and Computational Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [3]Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau Cedex, France

Magnetic excitations of the high-T_c cuprate superconductors (HTSC) are shown to be correctly reproduced within a two-dimensional Hubbard model in the appropriate strong-coupling regime. In particular, salient properties of the magnetic resonance mode, its intensity behavior in the underdoped regime and the "hour glass" dispersion display a good agreement with experiments. Our results are obtained in an essentially parameter-free theory based on an extension of the variational cluster approach (VCA) to treat two-particle excitations. When combined with earlier phase-diagram calculations using the VCA, it lends further support to a Hubbard-model description of the interplay of magnetism and superconductivity in the cuprate HTSC.