TT 16 Posters Correlated Electrons, Measuring Devices, Cryotechnique

Zeit: Samstag 11:00–16:30 Raum: Poster TU C

TT 16.1 Sa 11:00 Poster TU C

Quantum Criticality in the frustrated Laves phase compound $NbFe_2$ — •Dennis Moroni-Klementowicz, Manuel Brando, and Friedrich Malte Grosche — Department of Physics, Royal Holloway, University of London, Egham, TW20 OEX, United Kingdom

Geometric frustration in nearly magnetic metals provides a promising and relatively little explored path to obtaining high electronic density of states - hatching condition of novel quantum order. Various compounds close to the border of magnetism can be found amongst intermetallic C14 and C15 Laves phases. We have focused on one of the most interesting examples: $NbFe_2$. Depending on precise stoichiometry, pressure and applied magnetic field, $NbFe_2$ can be tuned between ferromagnetic, antiferromagnetic and enhanced paramagnetic low temperature states. Because stoichiometry and annealing are crucial in this compound we have put particular effort in making high quality samples using cold crucible RF heating techniques, extended annealing close to the melting point and zone refining, as well as detailed characterisation by heat capacity and magnetisation measurements. The complex phase diagram of $NbFe_2$ gives rise to several regions in which an ordering temperature is suppressed to low temperatures. We investigate the vicinity of these quantum critical points by high sensitivity measurements of the electrical resistivity under applied magnetic fields and high hydrostatic pressure, as well as ambient pressure heat capacity measurements, down to the sub-100 mK range.

TT 16.2 Sa 11:00 Poster TU C

Systematic Strong-Coupling Expansion of the T⊗t Jahn-Teller System — •Heinz Barentzen — Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart

Transition-metal oxides are notoriously difficult to describe because of a rather strong interplay between the spin, orbital and lattice degrees of freedom.This applies, in particular, to the recently investigated titanates with one t_{2g} electron per site, whose magnetic properties are surprising and controversial. Thus, e.g., while $YTiO_3$ shows a ferromagnetic ground state accompanied by a large Jahn-Teller (JT) distortion, $LaTiO_3$ exhibits an antiferromagnetic ground state with no detectable JT effect. To resolve the puzzling magnetic behavior of $LaTiO_3$, the concept of an orbital liquid has been worked out by Khaliullin et al.(Phys. Rev. Lett. **85**, 3950 (2000)), while a perturbing crystal field of the $GdFeO_3$-type has been proposed by Mochizuki and Imada (J. Phys.Soc.Jpn. **70**, 2872 (2001)).

To put these concepts on a quantitative basis we intend to elucidate the role of the T⊗t JT problem, relevant to these systems. So far, however, analytic results are available only for the limiting cases of weak and strong coupling. In an attempt to find the lowest eigenvalue of the T⊗t system over the whole coupling range, we have recently succeeded in obtaining systematic expansions for weak and strong coupling, the first steps on the way towards the complete solution of the problem. The reasoning behind these expansions will be explained and illustrated for the strong-coupling case.

TT 16.3 Sa 11:00 Poster TU C

Antiferromagnetic Quantum Chain Systems with Competing nn and nnn Interaction — •Reinhard K. Kremer — MPI für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

Antiferromagnetic (afm) S=1/2 Heisenberg chain systems with uniform nearest-neighbour exchange coupling are best understood. The ground state and the excitation spectrum are well known and the experimental observations are in good agreement with theory. Additional next-nearest neighbour exchange along the chains which can be described by the Majumdar-Ghosh Hamiltonian $H = J_{nn}\sum_i (S_iS_{i+1} + \alpha S_iS_{i+2})$ with α=J_{nnn}/J_{nn} gives rise to a more complex behaviour, since next-nearest neighbour interaction may lead to magnetic frustration. I review the magnetic properties of the afm S=1/2 Cu^{2+} chain systems $LiCuVO_4$ and CuX_2 (X=Cl, Br) for which afm *incommensurate* long-range ordering has been observed by neutron diffraction at low temperatures. The appearance of *incommensurate* ordering is ascribed to competing *nn* and *nnn* exchange interaction which is also evidenced in the bulk magnetic properties.

TT 16.4 Sa 11:00 Poster TU C

S=1 ground state in a hexacopper(II) molecular complex — •Volodymyr Pashchenko[1], Michael Lang[1], Bernd Wolf[1], Bernhard Brendel[1], Norbert Auner[2], Olga Shchegolikhina[3], and Yulia Molodtsova[3] — [1]Physikalisches Institut, J.W. Goethe-Universität, FOR 412, 60054 Frankfurt(M), Germany — [2]Institut für Anorganische Chemie, J.W. Goethe-Universität, 60439 Frankfurt(M), Germany — [3]A.N. Nesmeyanov Institute of Organoelement Compounds (INEOS), 28 Vavilov Str., 117813 Moscow, Russia

We report on an experimental determination by ESR of the molecular ground state in a hexacopper(II) siloxanolate compound. This system is distinct in that the six Cu^{2+} ions within the molecule are arranged in two almost parallel, linear trimers. According to magnetic measurements, the individual trimers couple antiferromagnetically with the dominant intratrimer exchange of J/k_B=85 K, yielding a spin-1/2 ground state at low temperatures. The weak intertrimer interactions of J'/k_B=−3 K appear to favor a ferromagnetic ground state for the molecules, with weak antiferromagnetic interactions between the molecules. Our low temperature single crystal ESR study clearly demonstrates that the molecular ground state of the complex is a triplet-singlet state, which is typical for an effective S=1 spin state. The data have been fitted by using the solutions of the spin Hamiltonian $\hat{H} = DS_z^2 + E(S_x^2 - S_y^2) + \mu_B \hat{g} BS$ with the parameters D=−0.30 cm^{-1}, E=−0.12 cm^{-1}, g_x=g_y=g_z=2.00 ± 0.05. It was found that the progressive formation of the molecular S=1 ground state occurs only below 40 K when the excited doublet and quartet states of individual trimers become completely thermally depopulated.

TT 16.5 Sa 11:00 Poster TU C

The Influence of Disorder and Thermal Fluctuations on 1d Density Waves and Luttinger Liquids — •Thomas Nattermann und Andreas Glatz — Institut für Theoretische Physik der Universität zu Köln, Zülpicher Str. 77, 50937 Köln

The low temperature phase diagram of 1D weakly disordered quantum systems like charge or spin density waves and Luttinger liquids is studied by a full finite temperature renormalization group (RG) calculation. For vanishing quantum fluctuations this approach is amended by an exact solution in the case of strong disorder and by a mapping onto the Burgers equation with noise in the case of weak disorder, respectively. At zero temperature we reproduce the quantum phase transition between a pinned (localized) and an unpinned (delocalized) phase for weak and strong quantum fluctuations, respectively, as found previously by Fukuyama or Giamarchi and Schulz.

At finite temperatures the localization transition is suppressed: the random potential is wiped out by thermal fluctuations on length scales larger than the thermal de Broglie wave length of the phason excitations. The existence of a zero temperature transition is reflected in a rich cross-over phase diagram of the correlation functions. The results can be transferred directly to the discussion of the influence of disorder in superfluids. Finally we extend the RG calculation to the treatment of a commensurate lattice potential. Applications to related systems are discussed as well.

TT 16.6 Sa 11:00 Poster TU C

Tomonaga-Luttinger-liquid parameter from density-matrix renormalization group calculations — •Satoshi Ejima[1], Florian Gebhard[1], and Satoshi Nishimoto[2] — [1]Fachbereich Physik, Philipps-Universität Marburg — [2]Institut für Theoretische Physik, Universität Göttingen

In a Tomonaga-Luttinger-liquid the density of states vanishes algebraically at the Fermi energy. The corresponding exponent α can be observed experimentally in quasi one-dimensional systems, e.g., in single-walled carbon nanotubes and other organic conductors. Experimental results, $\alpha > 1$, deviate substantially from those for simple one-dimensional models such as the Hubbard model where $\alpha \leq 1/8$. More realistic models contain nearest-neighbor interactions which strongly modify the critical exponent. However, the calculation of α for the extended Hubbard model is very difficult because no exact solution exists.

We use the density-matrix renormalization group (DMRG) method to calculate numerically the density-density correlation function for large systems with open boundary conditions. We extract α from the large-distance behavior of the density-density correlation function. We test

our approach against analytical results for the one-dimensional Hubbard model and the XXZ Heisenberg chain and find an excellent agreement. As an application we calculate α in the extended Hubbard model. We show that a lightly doped charge-density-wave insulator can exhibit $\alpha > 1$.

TT 16.7 Sa 11:00 Poster TU C

Influence of electronic correlations on the Drude response of two-dimensional organic conductors — •Natalia Drichko[1], Martin Dressel[1], Jaime Merino[2], and John Schlueter[3] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Universidad Autonoma de Madrid, Madrid, Spain — [3]Materials Science Division, Argonne National Laboratory, Argonne, USA

We use organic conductors as model objects to investigate the effects of reduced dimensions and electronic correlations. Conductivity in BEDT-TTF crystals occurs in the planes of the organic molecules, the overlap of the molecular orbitals defines the bandwidth W, the electronic correlations depend on the BEDT-TTF molecule parameters.

For the compounds α-(BEDT-TTF)$_2M$Hg(SCN)$_4$ (M=Rb, Tl, K, and NH_4) the structural parameters vary slightly, leading to an increase of ratio of electron-electron correlations to W on going from metallic Rb-salt to Tl, to K, and further to NH_4 (which becomes superconducting at $T_c \sim 1$ K). By measuring polarized reflection in the conducting plane of the crystals in the 8000-50 cm^{-1} range from $T = 300$ K to 5 K, we investigate how the electronic parameters depend on temperature and electronic correlations. The intensity of a Drude-peak increases below 50 K. The width of the Drude-component decreases when going from the Rb to the NH_4-compound, which we relate to the increase of electronic correlations. In addition, in the K-salt a pseudogap is observed around 100 cm^{-1} at T below 50 K, indicating charge-order fluctuations close to the superconducting state.

TT 16.8 Sa 11:00 Poster TU C

Tuning the Spin-State and Insulator-Metal Transition in $LaCoO_3$ by Eu-Doping — •J. Baier, M. Kriener, S. Jodlauk, A. Reichl, C. Zobel, H. Kierspel, A. Freimuth, and T. Lorenz — II. Physikalisches Institut, Universität zu Köln

We present a study of the structure, the electric resistivity, the magnetic susceptibility, and the thermal expansion of $La_{1-x}Eu_xCoO_3$ [1]. $LaCoO_3$ shows a temperature-induced spin-state transition around 100 K and a metal-insulator transition around 500 K. Partial substitution of La^{3+} by the smaller Eu^{3+} causes chemical pressure and leads to a drastic increase of the spin gap from about 190 K in $LaCoO_3$ to about 2000 K in $EuCoO_3$, so that the spin-state transition is shifted to much higher temperatures. A combined analysis of thermal expansion and susceptibility gives evidence that the spin-state transition has to be attributed to a population of a spin-triplet state, as is realized in the intermediate-spin state of Co^{3+}. In contrast to the spin-state transition, the metal-insulator transition is shifted only moderately to higher temperatures with increasing Eu content, showing that the metal-insulator transition occurs independently from the spin-state distribution of the Co^{3+} ions. Around the metal-insulator transition the magnetic susceptibility shows a similar increase for all x and approaches a doping-independent value around 1000 K indicating that well above the metal-insulator transition the same spin state is approached for all x.

[1] Baier *et al.*, cond-mat 0405680, appears in Phys. Rev. B

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TT 16.9 Sa 11:00 Poster TU C

Possible resolution of a temperature profile: A spin-chain study — •Markus Henrich, Michael Hartmann, and Günter Mahler — Institute of Theoretical Physics 1, University of Stuttgart

Possible spatial resolution of temperature profiles and their measurability have drawn increasing attention because of their relevance in recent experiments [1].

We investigate such a scenario in a simple quantum model: a spin-chain in contact with two heat baths at different temperatures. We study, under which conditions a local spin-temperature could exist in such spin-chains and how local a possible temperature measurement could be [2].

[1] P. Kim et al, Phys. Rev. Lett. 87/21, 215502 (2001).
[2] M. Hartmann et al, Phys. Rev. Lett. 93, 080402 (2004).

TT 16.10 Sa 11:00 Poster TU C

The Holstein-Hubbard Model away from Half-Filling — •Winfried Koller, Alex C. Hewson, and Dietrich Meyer — Department of Mathematics, Imperial College London

Recent experimental results in strongly correlated materials, such as fullerides, manganites and the high Tc compounds, have stimulated a renewed theoretical interest in the effects of electron-phonon interaction. The simplest model to examine the interplay of the electron-phonon and electron-electron interactions is Holstein-Hubbard model. This model has been predominantly studied under the assumption of particle-hole symmetry. Here we present results for the model away from half-filling using the dynamical mean-field theory in combination with the numerical renormalisation group. We calculate one-electron spectral densities and two-particle response functions. In particular, we examine the crossover from bipolaronic to polaronic behaviour, and compare our results with those derived from the many-body coherent-potential approximation (CPA).

TT 16.11 Sa 11:00 Poster TU C

Singular Dynamics of Underscreened Magnetic Impurity Models — •Winfried Koller, Alex C. Hewson, and Dietrich Meyer — Department of Mathematics, Imperial College London

We give a comprehensive analysis of the singular dynamics and of the low-energy fixed point of one-channel impurity s-d models with ferromagnetic and underscreened antiferromagnetic couplings. We use the numerical renormalization group (NRG) to perform calculations at $T = 0$. The spectral densities of the one-electron Green's functions and t-matrices are found to have very sharp cusps at the Fermi level ($\omega = 0$), but do not diverge. The approach of the Fermi level is governed by terms proportional to $1/\ln 2(\omega/T_0)$ as $\omega \to 0$. The scaled NRG energy levels show a slow convergence as $1/(N + C)$ to their fixed point values, where N is the iteration number and C is a constant dependent on the coupling J from which the low energy scale T_0 can be deduced. We calculate also the dynamical spin susceptibility, and the elastic and inelastic scattering cross-sections as a function of ω. The inelastic scattering goes to zero as $\omega \to 0$, as expected for a Fermi liquid, but anomalously slowly compared to the fully screened case. We obtain the asymptotic forms for the phase shifts for elastic scattering of the quasiparticles in the high-spin and low-spin channels.

TT 16.12 Sa 11:00 Poster TU C

Quantenphasenübergang im spinlosen Holstein-Modell — •Steffen Sykora[1], Arnd Hübsch[1,2] und Klaus W. Becker[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden — [2]Department of Physics, University of California, Davis, CA 95616, USA

Mit Hilfe des Projektor-basierten Renormierungsverfahrens (PRM) wird der Metall-Nichtmetall-Quantenphasenübergang im eindimensionalen Holstein-Modell bei Halbfüllung untersucht. In dem PRM-Verfahren werden sukzessiv hochenergetische Anregungsoperatoren der Elektron-Phonon-Wechselwirkung herausintegriert. Als Ergebnis erhält man einen effektiven Hamiltonoperator für ein quasifreies System aus renormierten ungekoppelten Elektronen und Phononen. Für Werte der Elektron-Phonon-Kopplung g oberhalb eines kritischen Wertes g_c befindet sich das System in einem geordneten Zustand entsprechend einer isolierenden Peierls-Phase. In dieser Arbeit wird das Verhalten der renormierten Ordnungsparameter für die Peierls-Gitterverzerrung $\tilde{\Delta}^b$ und die Ladungsdichtewelle $\tilde{\Delta}^c_k$ in Abhängigkeit von g für beide Phasen untersucht. Desweiteren wird für den gesamten Parameterbereich von g die renormierte Phononenfrequenz $\tilde{\omega}_q$ und die elektronische Einteilchenenergie $\tilde{\varepsilon}_k$ berechnet. Wird der quantenkritische Punkt g_c überschritten, so öffnet sich eine Lücke an der Fermikante im elektronischen Anregungsspektrum, was dem Übergang von der metallischen in die isolierende Phase entspricht.

TT 16.13 Sa 11:00 Poster TU C

Dynamic charge and spin susceptibility of the Hubbard model — •Sebastian Schmitt and Norbert Grewe — Institut für Festkörperphysik, Hochschulstraße 6, 64289 Darmstadt

We present Bethe-Salpeter equations, derived via a cumulant expansion in terms of the transfer between lattice sites, which are valid for models with large local Coulomb matrix elements. Employing a RPA-like decoupling scheme, susceptibilities of a Stoner form are obtained, in which the local parts and their dynamic interactions are explicitly known.

For the Hubbard model the dynamic charge and spin susceptibility is presented and discussed. In particular the spectra of charge and spin fluctuations are analyzed as well as tendencies towards the formation of a charge or magnetically ordered state for various wave vectors, temperatures, and doping.

TT 16.14 Sa 11:00 Poster TU C

Electronic Phase Separation in $La_{1-x}Sr_xMnO_3$ films, x $\tilde{1}$/8. — •Peter Wochner[1], U. Gebhardt[1], A. Vigliante[2], N. Kasper[1], J. Geck[3], H.U. Habermeier[4], and F. Razavi[5] — [1]MPI f. Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — [2]Bruker AXS GmbH, Karlsruhe — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden — [4]MPI f. Festkörperforschung, Stuttgart — [5]Brock University, St. Catherines, Ontario, Canada

Recently, it was shown by J. Geck et al. that the low temperature ferromagnetic and insulating phase of bulk $La_{7/8}Sr_{1/8}MnO_3$ can be explained by an ordering of orbitals and holes in form of an orbital polaron lattice. Films of the same material on $SrTiO_3 < 001 >$ oriented substrates show a metal-insulator transition for thicknesses smaller $\tilde{5}$00 A. Thicker films are insulators at low temperature. By synchrotron X-ray diffraction we found in these films one of the signatures of the orbital polaron (OP) phase which indicates the presence of half doped charge stripes together with a structural modulation. This OP phase is only short-range ordered and coexists with the antiferro-orbital ordered matrix.

TT 16.15 Sa 11:00 Poster TU C

Anomaloos high ordering temperature in $YbRu_2Ge_2$ — •H. S. Jeevan[1], Z. Hossain[1,2], and C. Geibel[1] — [1]MPI-CPfS Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Department of Physics, I.I.T-Kanpur, 208016. India

In search for new Yb-base stoichiometric systems which are close to quantum critical point at ambient pressure, we have synthesized and investigated single crystals of $YbRu_2Ge_2$, an homologue of$YbRh_2Si_2$. From the systematic of the known YbM_2X_2 (M = d elements, X = Si, Ge) we had hoped that this compound will be nonmagnetic and located close to a QCP. But surprisingly we found that in $YbRu_2Ge_2$, Yb is in a stable trivalent state and present some kind of ordering at a much higher temperature T_M =10K then in presently known Yb-compounds. High temperature magnetic susceptibility follows Curie-Weiss behavior with effective moment very close to that expected for trivalent Yb ions. Low temperature susceptibility exhibits a peak at 6 K presumably due to antiferromagnetic type of order. Resistivity linearly decreases with temperature down to about 50 K, then increases with further decreasing temperature due to Kondo interaction, passes though a maximum at 10 K below which the resistivity undergoes a rapid decrease due to freezing out of spin disorder scattering. The Specific heat of $YbRu_2Ge_2$ shows two large peaks, one at 10K and another at 6K, the low temperature anomaly corresponding to the antiferromagnetic transition as detected by χ(T). The nature of the high temperature anomaly in specific heat is under investigation.

TT 16.16 Sa 11:00 Poster TU C

Crossover from Single-Ion to Coherent Non-Fermi Liquid Behavior in $Ce_{1-x}La_xNi_9Ge_4$ — •E.-W. Scheidt[1], U. Killer[1], H. Michor[2], S. Kehrein[3], and W. Scherer[1] — [1]CPM, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — [2]Institut für Festkörperphysik, TU Wien, 1040 Wien, Austria — [3]TP III – EKM, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

We report specific heat , susceptibility and resistivity studies on the compound $Ce_{1-x}La_xNi_9Ge_4$ for various concentrations ranging from the stoichiometric system with $x = 0$ to the dilute limit $x = 0.95$ [1]. Our data reveal single-ion scaling with the Ce-concentration and the largest ever recorded value of the electronic specific heat $\Delta c/T \approx 5.5\, JK^{-2}mol^{-1}$ at $T = 0.08$ K for the stoichiometric compound at $x = 0$ without any trace of magnetic order. While in the doped samples $\Delta c/T$ and ρ increase logarithmically in the range between 3 K and 50 mK and between 20 K and 5 K, respectively, their magnetic susceptibility behaves Fermi liquid like below 1 K. $\Delta c/T$ in $CeNi_9Ge_4$ flattens out below 200 mK and displays a pronounced maximum in the resistivity curve at 4K indicating a coherent heavy fermion groundstate [2]. These properties render the compound $Ce_{1-x}La_xNi_9Ge_4$ a unique system on the borderline between Fermi liquid and non-Fermi liquid physics. [1] U. Killer, E.-W. Scheidt, G. Eickerling, H. Michor, J. Sereni, Th. Pruschke, S. Kehrein, Phys. Rev. Let. (cond-mat/0402498), in print. [2] E.-W. Scheidt, U. Killer, H. Michor, E. Bauer, C.Dusec, S. Kehrein and W. Scherer, Physika B, in print.

TT 16.17 Sa 11:00 Poster TU C

Thermal transport properties of $YbRh_2(Si_{1-x}Ge_x)_2$ at low temperatures — •Stefanie Hartmann, Adriana Sanchez, Silke Paschen, Octavio Trovarelli, Christoph Geibel, and Frank Steglich — MPI CPfS, Nöthnitzer Str. 40, 01187 Dresden

The heavy-fermion compound $YbRh_2Si_2$ orders antiferromagnetically at $T_N = 70$ mK and reveals non-Fermi liquid behavior in the vicinity of a (magnetic-field induced) quantum critical point [1,2]. Here we present thermal transport properties of pure and 5% Ge-doped samples. The previously reported logarithmic temperature dependence of the electronic specific heat coefficient C_{el}/T between 0.3 and 10 K [2] is reflected in the thermal conductivity over temperature ratio κ/T. The electronic contribution of κ shows deviations from the predictions of the Wiedemann-Franz law based on calculations from resistivity measurements. Thus, the applicability of the WF law seems to be questionable. The logarithmic behavior of $C_{el}(T)/T$ is also observed in the thermopower over temperature ratio $S(T)/T$ as theoretically predicted by Paul et al. [3]. But below 2 K S/T exhibits a stronger than logarithmic divergence ("upturn") with decreasing temperature.

[1] P. Gegenwart et al., PRL 89, 056402 (2002)
[2] J. Custers et al., Nature 424, 524 (2003)
[3] I. Paul and G. Kotliar, PRB 64, 184414 (2001)

TT 16.18 Sa 11:00 Poster TU C

Tetracritical point in $CeCu_2(Si_{1-x}Ge_x)_2$ investigated by neutron diffraction — •Enrico Faulhaber[1], Oliver Stockert[2], Beatrice Grenier[3], Bachir Ouladdiaf[3], Micha Deppe[2], Christoph Geibel[2], Frank Steglich[2], and Michael Loewenhaupt[1] — [1]Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — [2]Max-Planck-Institut für Chem. Physik fester Stoffe, D-01187 Dresden, Germany — [3]Institut Laue-Langevin, F-38042 Grenoble, France

The heavy-fermion system $CeCu_2(Si_{1-x}Ge_x)_2$ attracts not only interest close to $x = 0$ with the interplay of antiferromagnetism and superconductivity in pure $CeCu_2Si_2$, but also in the vicinity of $x = 0.25$ where the antiferromagnetic order is suggested to change from a spin-density wave to a more localized type of magnetic order. Moreover, specific heat as well as thermal expansion measurements indicate the possible existence of a tetracritical point at $x \approx 0.25$. For higher and lower Ge concentrations exists a first order transition below the Néel temperature, whereas for $x = 0.25$ both transitions seem to be degenerate. Furthermore, the anomalies in the thermal expansion have opposite signs below and above $x = 0.25$ suggesting a different magnetic stucture. We performed extensive neutron diffraction on $CeCu_2(Si_{1-x}Ge_x)_2$ single crystals with $x = 0.16$ and 0.45, i.e. on either site of $x = 0.25$. Both samples show antiferromagnetic order with slightly different propagation vectors followed by a lock-in transition. This suggests a modified nesting of the Fermi surface. The magnetic structure will be discussed in comparison to macroscopic measurements.

TT 16.19 Sa 11:00 Poster TU C

Distribution of the Kondo temperature in strongly coupled two-level systems: an NRG study — •Christian Kolf — kolf@th.physik.uni-bonn.de

Conductance measurements on quantum point contacts show zero-bias anomalies in the differential conductance which are consistent with the presence of two-channel Kondo (2CK) impurities and which are difficult to explain by any other known microscopic mechanism. The 2CK effect has been proposed by degenerate two-level systems. As one of the unresolved problems within the two-channel Kondo scenario, however, the experimental results indicate a very narrow distribution of the Kondo temperature T_K, $P(T_K)$. We argue by general renormalization group arguments that a wide distribution of the Kondo coupling constant J – which is expected for a nanoscopic point contact – leads to a peaked distribution of the resulting T_K, if the distribution of J extends beyond the region $J \ll D$ where D is the characteristic high energy scale, i.e. the band width. We investigate the distribution $P(T_K)$ by means of explicit numerical renormalization group (NRG) calculations.

TT 16.20 Sa 11:00 Poster TU C

Multi-level Kondo effect in single-wall carbon nanotubes (SWNT) — •Theresa Hecht, Michael Sindel und Jan von Delft — Department of Physics and Center for NanoScience, LMU München, Theresienstr. 37, 80333 München

Recently Herrero et al. investigated the Kondo effect [1] in SWNTs. In absence of a magnetic field an (approximate) orbital as well as a spin degeneracy is present in those SWNT. Herrero et al. were able to identify two consequences of this degeneracy, namely the so-called SU(4) Kondo effect [2] and a purely orbital Kondo effect [3]. A finite magnetic field was found to remove both spin and orbital degeneracy, reflected by multiple splittings of the Kondo resonance. Moreover, a particular magnetic field

might even result in a degeneracy between adjacent orbital levels, giving rise to a purely orbital Kondo effect [3]. In some samples, the Kondo resonance is split even in the complete absence of a magnetic field, suggesting that the orbital states are weakly coupled, lifting their degeneracy.

Motivated by these experiments, we study a two-level Anderson model by means of Wilson's numerical renormalization group method. We investigate both magnetic field and energy dependence of the spectral function and propose a mechanism that leads to the various types of splittings of the Kondo resonance.

[1] P. Jarillo-Herrero et al., submitted to Nature
[2] L. Borda et al., PRL 90, 026602, (2003)
[3] P. Jarillo-Herrero et al., to be published

TT 16.21 Sa 11:00 Poster TU C

Phase Transitions in the Pseudogap Anderson and Kondo models — •Lars Fritz, Marijana Kircan, and Matthias Vojta — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe,76128 Karlsruhe

The Pseudogap Kondo problem, describing quantum impurities coupled to fermionic quasiparticles with a pseudogap density of states, $\rho(\omega) \propto |\omega|^r$, shows a rich zero-temperature phase diagram, with different screened and free moment phases and associated transitions. We analyze both the particle-hole symmetric and asymmetric cases using renormalization group techniques. In the vicinity of $r = 0$, which plays the role of a lower critical dimension, an expansion in the Kondo coupling is appropriate. In contrast, $r = 1$ is the upper-critical dimension in the absence of particle-hole symmetry, and here insight can be gained using an expansion in the hybridization strength of the Anderson model. As a by-product, we show that the particle-hole symmetric strong coupling fixed point for $r < 1$ is described by a resonant level model, and corresponds to an intermediate-coupling fixed point in the renormalization group language. Interestingly, the value $r = \frac{1}{2}$ plays the role of a second lower-critical dimension in the particle-hole symmetric case, and there we can make progress by a novel expansion performed around a resonant level model. The different expansions allow a complete description of all critical fixed points of the models and can be used to compute a variety of properties near criticality, describing universal local-moment fluctuations at these impurity quantum phase transitions.

TT 16.22 Sa 11:00 Poster TU C

Magnetic field dependence of the electronic phase coherence length of diffusive nanowires with magnetic impurities — •Christian Schirm[1], Elke Scheer[1], Christian Paschke[2], Christoph Sürgers[2], and Hilbert v. Löhneysen[2] — [1]Fachbereich Physik, Universität Konstanz, D-78464 Konstanz — [2]Physikalisches Institut and DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe

For the study of the electronic phase coherence length l_φ of diffusive metal structures at very low temperatures, Mohanty et al. [1] propose to investigate the conductance fluctuations (CF) at high magnetic fields. The authors claim that the possible presence of small amounts of magnetic impurities should be detectable by analyzing the field dependence of the fluctuations. In [2] the CF of diffusive Cu nanowires, intentionally contaminated with Mn impurities in the ppm range, were investigated. We had observed a complex field and concentration dependence of l_φ. We re-evaluated the data of [2] with a refined numerical treatment. The influence of the signal to noise ratio (SNR) of the conductance measurements on the determination of l_φ is discussed. Although the SNR in [2] is of the same order or better than in [1] we obtain a wide range of possible values for l_φ depending on the treatment of the background and other numerical or physical parameters. Thus, the absence of a magnetic field dependence of l_φ cannot be taken as evidence against the presence of magnetic impurities limiting l_φ for $T \to 0$.

[1] P. Mohanty et al., Phys. Rev. Lett. 91, 066604 (2003)
[2] H. v. Löhneysen et al., Physica B 284-288, 1858 (2000)

TT 16.23 Sa 11:00 Poster TU C

Self-energy near Pomeranchuk instability — •Luca Dell'Anna and Walter Metzner — Max Planck Institut fuer FKF, D-70569 Stuttgart

Electron-electron interaction can induce Fermi surface deformations. We study the decay rate behavior for single particle excitations near d-wave Pomeranchuk instability in two dimensions.

TT 16.24 Sa 11:00 Poster TU C

Delocalization of electrons in disordered films induced by parallel magnetic field and film thickness — •R.K. Brojen Singh, V.Z. Cerovski, and M. Schreiber — Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

We present results of the investigation of delocalization of non-interacting electrons in disordered thin films induced by parallel magnetic field B and film thickness b. We compare two procedures within the framework of self-consistent theory of localization for weak fields generalized to situations lacking time reversal invariance by (a) taking the diffusion constants, D^{pp} and D^{ph} corresponding to particle-particle and particle-hole channels respectively as equal, and (b) taking $D^{pp} \neq D^{ph}$. The two procedures give different results, the main one being that (a) gives the metal-insulator transition (MIT) at $T = 0$ induced by the magnetic field and film thickness, but (b) does not. In the insulating regime we find the localization length as a function of B, b and λ (disorder strength) and calculate critical values of B, b and λ. In the metallic regime we calculate conductivity as a function of these parameters. At $T > 0$ both procedures give an MIT.

TT 16.25 Sa 11:00 Poster TU C

Density of states of the three dimensional Bernoulli-Anderson model — •P. Karman, V. Z. Cerovski, and M. Schreiber — Institut für physik, Technische Universität Chemnitz, D-09107 Chemnitz

The density of states of the Bernoulli-Anderson model, defined as the tight-binding Hamiltonian of non-interacting electrons with disorder introduced by the random distribution of only two on-site energies, is studied using the large scale numerical diagonalization of Hamiltonians. In particular, we determine the band structure and the propreties of the band tail states and compare the results with the Anderson model of disorder.

TT 16.26 Sa 11:00 Poster TU C

Metal-insulator transition in quasi-2D systems — •K. Morawetz — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

The conductivity in quasi two-dimensional systems is calculated using the quantum kinetic equation. The system of quasi two-dimensional electrons in hetero-junctions which interact with charged and neutral impurities and the low temperature correction to the conductivity is calculated analytically. It turns out that the dynamical screening due to charged impurities leads to a linear temperature dependence, while the scattering from neutral impurities leads to the usual Fermi-liquid behavior. The experimental metal-insulator transition at low temperatures are reproduced [1]. The effective mass of quasiparticle excitations in quasi two-dimensional systems is calculated analytically. It is shown that the effective mass increases sharply when the density approaches the critical one of metal-insulator transition. This suggests a Mott-type of transition rather than an Anderson-like transition [2].

[1] K. Morawetz, Phys. Rev. B 67 (2003) 115125
[2] K. Morawetz, Europhys. Lett. 67 (2004) 77–83

TT 16.27 Sa 11:00 Poster TU C

Optical studies of the bandwidth controlled Mott-Hubbard transition in 2-dim organic charge transfer salts. — •Daniel Faltermeier, Michael Dumm, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

The quasi two-dimensional organic charge-transfer salts κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br$_x$Cl$_{1-x}$ have attracted lots of interest because of their unique physical properties: by applying moderate external pressure or by alloying with Br or Cl the ground state can be switched between an antiferromagnetic insulating and superconducting state. In contrast to the high-T$_c$ cuprates the Mott-Hubbard-transition is achieved by bandwidth control and not by hole doping. We present polarization dependent reflection data of the κ-(BEDT-TTF)$_2$ salts in a spectral range from 50 to 8000 cm^{-1} with different concentration x of Br and in a temperature range from 5 to 300 K. Starting from the pure Cl component, with increasing Br concentration and decreasing the temperature, the material becomes continuously more and more metallic, what is characterized by a strong Drude tail at low frequencies. Furthermore, we present detailed analysis of the optical conductivity in the vicinity of the insulator-to-metal transition including e.g. the broad absorption hump in the mid-infrared region.

TT 16.28 Sa 11:00 Poster TU C

Metal-insulator transition in the Hubbard Model at finite doping and temperature — •Rolf Helmes, Achim Rosch, and Theo Costi — Institut für Theoretische Physik, Universität zu Köln

The dynamical mean field theory in combination with the numerical renormalization group is used to compute the phase diagram of the Hubbard model away from half-filling in the (T,U) plane. We find regions of coexistance of two solutions with the same doping at finite temperature, as for half filling. In addition we find regions of phase-separation. We discuss the effect of particle-hole asymmetry on the phase diagram at half-filling, and the influence of a small doping on the single-particle spectra of a Mott insulator.

TT 16.29 Sa 11:00 Poster TU C

The Role of Power-Law Correlated Disorder in the Anderson Metal-Insulator Transition — •A. Croy, V. Z. Cerovski, and M. Schreiber — Institut für Physik, Technische Universität, 09107 Chemnitz, Germany

The effect of long-range correlations of the form $g(r) \propto r^{-\alpha}$ in classical systems, such as site or bond percolation problems, is well understood in terms of the *extended Harris criterion* [1]. It predicts a critical value $\alpha_c = 2/\nu_0$ for the correlation strength, below which the correlations become relevant and the critical exponent changes from ν_0 to $\nu = 2/\alpha$. The question whether this criterion still holds for quantum systems is still under investigation. Recent results for ν in the Anderson model of localization in 3d suggest such a behavior for fixed disorder strength W, but not for a fixed energy $E = 0$ at the band center [2]. We present results of the dependence of ν on α for both fixed W and fixed E, obtained using the finite size scaling of the largest inverse Lyapunov exponent of the transfer matrices of long quasi-1d systems.

[1] A. Weinrib, Phys. Rev. **B29**, 387 (1984)
[2] M. L. Ndawana, R. A. Römer and M. Schreiber, Europhys. Lett., Published online: 5 November 2004, doi:10.1209/epl/i2004-10267-5

TT 16.30 Sa 11:00 Poster TU C

Hubbard model in a magnetic field at weak coupling — •Carsten Knecht and P.G.J. van Dongen — Institut fuer Physik, Universitaet Mainz

The phase diagram of the half-filled Hubbard model is studied at weak coupling in two spatial dimensions. A homogeneous magnetization in the z-direction and a staggered magnetization in the x-direction are assumed. We apply perturbation theory at fixed order parameter (PTFO) to this system. The results are compared with the well know Hartree-Fock solutions that usually overestimate the order parameters. This calculation is also relevant for superconductivity in the doped two-dimensional negative-U Hubbard model.

TT 16.31 Sa 11:00 Poster TU C

Exact diagonalization studies of hole-doped spin rings — •Fatiha Ouchni and Jürgen Schnack — Universität Osnabrück, Fachbereich Physik, D-49069 Osnabrück, Germany

Motivated by the effect of holes on the electric and magnetic properties of the spin-chain and -ladder compound $Sr_{14}Cu_{24}O_{41}$, we study the influence of the Coulomb repulsion between different holes on the ring using exact diagonalization of an extended Hubbard model via a Lanczos procedure. The resulting correlation functions depend strongly on the strength and the range of the screened Coulomb potential. It is shown that strong Coulomb repulsion leads to well-localized holes and very likely to a dimerized ground state in the case of 60 % intrinsic hole doping.

TT 16.32 Sa 11:00 Poster TU C

Structural and magnetic investigations on new molecular quantum rings — •Volodymyr Pashchenko[1], Michael Lang[1], Bernd Wolf[1], Larisa Zherlitsina[2], Norbert Auner[2], Olga Shchegolikhina[3], and Yulia Pozdniakova[3] — [1]Physikalisches Institut, J.W. Goethe-Universität, FOR 412, 60054 Frankfurt(M), Germany — [2]Institut für Anorganische Chemie, J.W. Goethe-Universität, 60439 Frankfurt(M), Germany — [3]A.N. Nesmeyanov Institute of Organoelement Compounds (INEOS), 28 Vavilov Str., 117813 Moscow, Russia

Three oxygen-bridged polynuclear Cu(II) (N=6,8,10) cyclosiloxanolate complexes, $[Cu_6(MeSiO_2)_{12}]\cdot 6DMF$, $\{[Cu_8(MeSiO_2)_{16}]\cdot 8DMF\}\cdot EtOH$ and $\{[Cu_{10}(MeSiO_2)_{20}]\cdot 10DMF\}\cdot 6DMF$, have been synthesized and characterized structurally and magnetically. All three molecule-based complexes exhibit a similar structure consisting of rings of N=6, 8 or 10 Cu(II) atoms sandwiched by two N-membered cyclomethylsiloxanolate ligands. Within the rings, adjacent Cu^{2+} ions are linked by pairs of siloxanolate oxygen atoms which provide the magnetic exchange path for the Cu(II) S=1/2 spins. A detailed analysis of the magnetic properties reveals a strong ferromagnetic Cu-Cu exchange interaction (J/k_B=−62 K) for the N=6 compound with an S=3 high-spin ground state, a moderately strong ferromagnetic interaction (J/k_B=−27.6 K) for N=8 and an antiferromagnetic interaction (J/k_B=+17.2 K) with a nonmagnetic S=0 ground state for N=10. These results together with structural investigations enable to correlate structural parameters such as the Cu-O-Cu bridging angle with the sign and strength of the magnetic exchange coupling J.

TT 16.33 Sa 11:00 Poster TU C

Charge Transport Through Quench-Condensed Hydrogen Films — •Jörg Angrik, Patrick Schwinzer, Jürgen Klier, and Paul Leiderer — Fachbereich Physik, Universität Konstanz, Postfach M676, D-78457 Konstanz

The self-charging of quench-condensed tritium films prevents their use as a source in the next generation direct neutrino mass experiments. The KATRIN experiment, which is set up at the Forschungszentrum Karlsruhe, is the successor of the Mainz neutrino mass experiment, where such films were used. As the resolution of the KATRIN experiment will be in the sub-eV range, the self-charging effect cannot be tolerated. While the mobility of positive charges ($^3He^+$, originating from the β-decay) is well understood in terms of a thermal hopping model in a critical electric field ($E_c \approx 62\,\mathrm{MV/cm}$ at 1.9 K), little is known about the transport of negative charges. Hence we place electrons on top of hydrogen films, which then form surface states, and investigate their transport through the films. Hereby hydrogen, and also deuterium, are used to model the tritium films. As the transport is supposed to be strongly dependent on the structure of the, e.g., quench-condensed, films, we focus on preparation procedures and treatments in order to increase the conductivity of the electrons or discharge of the films.

TT 16.34 Sa 11:00 Poster TU C

Optical studies on the two-leg ladder compounds $Sr_{14-x}Ca_xCu_{24}O_{41}$ under pressure — •S. Frank[1], R. Klingeler[2], B. Büchner[2], and C. A. Kuntscher[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, PF 27 01 16, 01171 Dresden, Germany

The low-dimensional quantum spin system $Sr_{14}Cu_{24}O_{41}$, composed of planes consisting of edge-sharing CuO_2 chains and planes of two-leg Cu_2O_3 ladders, has been studied extensively because of its interesting electronic and magnetic properties. Its electronic characteristics and the distribution of charges among the various structural entities are influenced by Ca-doping. The most interesting phenomenon in $Sr_{14}Cu_{24}O_{41}$ is a superconducting phase for high Ca-doping and under high pressure. Pressure-dependent resistivity measurements on $Sr_{2.5}Ca_{11.5}Cu_{24}O_{41}$ [1] suggest the occurrence of a dimensional crossover from one to two under pressure, and that the superconductivity in this system is essentially a 2D phenomenon.

We carried out polarization-dependent RT reflectivity measurements on $Sr_{14-x}Ca_xCu_{24}O_{41}$ single crystals, with x=4 and 11.5, as a function of pressure (<20 GPa). The results are discussed in terms of changes in the charge dynamics along and perpendicular to the ladders and a possible pressure-induced dimensional crossover. *Supported by the DFG, Emmy Noether-program.*

[1] T. Nagata *et al.*, Phys. Rev. Lett. **81**, 1090 (1998).

TT 16.35 Sa 11:00 Poster TU C

NMR Untersuchungen der Spindiffusion in den Spinleitern von $Sr_{14}Cu_{24}O_{41}$ — •A. Bosse[1], M.S. Rose[2], L. Shu[2], D.E. MacLaughlin[2], R. Klingeler[3], B. Büchner[3], F.J. Litterst[1] und H.-H. Klauss[1] — [1]Institut für Metallphysik und Nukleare Festkörperphysik, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig — [2]Department of Physics, University of California Riverside, CA 92521, USA — [3]Institut für Festkörperforschung, IFW Dresden, Helmholtzstr. 20, 01069 Dresden

In dem eindimensionalen S = $\frac{1}{2}$ Quantenspinsystem $Sr_{14}Cu_{24}O_{41}$, das Cu_2O_3 Spinleitern enthält, wurde eine außergewöhnlich hohe thermische Leitfähigkeit entlang der Kettenrichtung beobachtet, die auf Spinanregungen zurückgeführt wird [1]. Wir haben Messungen der longitudinalen

NMR- Relaxationsrate an den ^{63}Cu- Kernen der Spinleiter als Funktion der Temperatur und des externen Magnetfelds durchgeführt. Es ergibt sich ein Anstieg der Spindiffusion im Temperaturregime der Spinanregungslücke. Die Ergebnisse werden im Hinblick auf einen Zusammenhang mit der thermischen Leitfähigkeit diskutiert.

[1] C. Hess, H. ElHaes, B. Büchner, U. Ammerahl, M. Hücker, A. Revcolevschi, PRL 93 (2004), 027005

TT 16.36 Sa 11:00 Poster TU C

Heat transport in S=1/2 spin ladders and chains — •C. Hess[1], P. Ribeiro[1], H. ElHaes[2], G. Roth[2], C. Sekar[1], G. Krabbes[1], B. Büchner[1], F. Heidrich-Meisner[3], W. Brenig[3], M. Hücker[4], U. Ammerahl[4], and A. Revcolevschi[4] — [1]IFW Dresden, Germany — [2]RWTH Aachen, Germany — [3]Institut für Theoretische Physik, TU-Braunschweig, Germany — [4]Laboratoire de Physico-Chimie des Solides, Université Paris-Sud, France

We present experimental results for the magnon thermal conductivity $\kappa_{\rm mag}$ of several one-dimensional S=1/2 spin systems, like spin ladders and chains. We discuss in detail the different scattering mechanisms of magnons in the spin ladder system $(Sr, Ca, La)_{14}Cu_{24}O_{41}$, i.e. scattering on static defects, phonons, magnons and holes. We compare these results with the magnetic heat transport in the anisotropic ladder compound $CaCu_2O_3$ and the spin chain material $(Sr, Ca)CuO_2$.

TT 16.37 Sa 11:00 Poster TU C

Triplet excitations of bond-disordered spin-1/2 ladders — •Marcelo Arlego[1,2], Wolfram Brenig[1], Daniel Cabra[3], Fabian Heidrich-Meisner[1], Andreas Honecker[1], and Gerardo Rossini[3,2] — [1]Technische Universität Braunschweig, Institut für Theoretische Physik, Mendelssohnstraße 3, 38106 Braunschweig, Germany — [2]Universidad Nacional de La Plata, Departamento de Fisica, C.C. 67, (1900) La Plata, Argentina — [3]Université Louis Pasteur, Laboratoire de Physique Théorique, 3 Rue de l'Université, 67084 Strasbourg Cedex, France

We analyze the effect of weak bond disorder in two-leg spin ladders, focusing on the appearance of bound states in the spin gap. Performing a projection on the single-triplet subspace we analytically derive the position of bound states for single-impurity and small impurity clusters in the strong-coupling limit, i.e., strong dimerization. Both the case of modified exchange couplings on the rungs and on the legs of the ladder are studied. Numerically, we analyze the single-impurity problem in a spin ladder by the Lanczos method to obtain the low-lying excitations. The case of a finite concentration of impurities is treated to leading order in the interung coupling within the single-triplet subspace by numerical impurity averaging of large systems. We compare the spectra obtained numerically with the results of diagrammatic techniques, particularly the coherent-potential approximation (CPA). Since the CPA does not account for the interference of impurities we discuss the contribution of small impurity clusters to the density of states.

TT 16.38 Sa 11:00 Poster TU C

Anisotropic thermal transport in one-dimensional spin systems — •K. Kordonis[1], T. Lorenz[1], A. Freimuth[1], Y. Ueda[2], M. Isobe[2], A. Vasil'ev[3], and S. Cheong[4] — [1]II. Phys. Inst., Universität zu Köln — [2]Inst. Sol. St. Phys., University of Tokyo — [3]Low Temp. Phys. Dep., Moscow State University — [4]Dep. of Phys. & Astron., Rutgers University

One-dimensional spin systems show unusual and rich physical properties. Of particular interest are the dynamics of magnetic excitations and their coupling to the lattice. A valuable tool for their study is provided by measurements of the thermal conductivity κ. We present measurements of κ of the spin-ladder system α-NaV_2O_5, of the spin-chain systems β-$Na_{0.33}V_2O_5$, LiV_2O_5 and the Haldane system Y_2BaNiO_5. A double-peak structure of κ versus T is obtained in both sodium vanadates along and perpedicular to the magnetic directions. The origin of these double peaks is ambiguous yet, but the isotropic behavior of κ concerning different lattice directions is evidence for a phononic thermal conductivity. The minimum of κ can be explained by damping close to the transition temperature. In LiV_2O_5, κ shows only one low-temperature maximum along and perpedicular to the chains. Accordingly, κ of the vanadates is purely phononic. In contrast, κ of Y_2BaNiO_5 behaves strongly anisotropic; a double-peak of κ versus T is obtained only along the spin chains. This is a clear evidence for an additional magnetic contribution to the thermal conductivity of the Haldane system.

supported by the DFG through SFB 608

TT 16.39 Sa 11:00 Poster TU C

The use of hydroquinone-derived linkers for the design of low-d spin systems: from isolated dimers to Heisenberg chains — •Bernd Wolf[1], Andreas Brühl[1], Jörg Magerkurth[1], Volodymyr Pashchenko[1], Bernhard Brendel[1], Michael Lang[1], Günter Margraf[2], Hans-Werner Lerner[2], Tonia Kretz[2], and Mathias Wagner[2] — [1]Physikalisches Institut, Universität Frankfurt, 60054 Frankfurt, FOR 412 (Germany) — [2]Institut für Anorganische Chemie,

In the course of an interdisciplinary research program to synthesize new classes of molecule-based quantum magnets which enable their fundamental physical properties to be explored systematically upon variations of physical or chemical parameters, we have produced a series of low-dimensional quantum-spin systems. The materials are all based on hydroquinone-derived linkers connecting Cu^{2+} ions carrying a spin of S = 1/2. The measurements of magnetic, magnetothermal and magnetoelastic properties cover wide ranges of temperatures 0.06 K < T < 320 K and magnetic fields B < 50 T. Especially for a 1-D Heisenberg antiferromagnet with a moderate magnetic coupling constant we have been able to perform experiments across the saturation field $g\mu_B B_S = 2|J|$ which marks, at T = 0, the endpoint of a quantum-critical line in the B-x plane. It has been found that crossing B_S is accompanied by a distinct magnetocaloric effect. In addition, a pronounced acoustic anomaly has been observed close to B_S and identified as a generic property of the uniform antiferromagnetic Heisenberg chain with a finite spin-lattice coupling.

TT 16.40 Sa 11:00 Poster TU C

Bosonization of dimerized Hubbard chains — •Carmen Mocanu, Peter Schwab, Michael Dzierzawa, and Ulrich Eckern — Institut für Physik, Universität Augsburg, 86135 Augsburg

The foundations of bosonization were laid more than 50 years ago in a seminal paper by Tomonaga. During the following decades the method has been worked out and successfully applied to one-dimensional electron and spin systems. Despite its long history there are still some subtle points in the bosonization formalism which are not taken into consideration in the majority of the literature. One of these issues is the proper treatment of the so-called Klein factors which have to be introduced in order to preserve the anticommuting property of the fermionic fields during the bosonization procedure.

In our approach we handle the Klein factors in a systematic way, both in the thermodynamic limit and for finite systems, using a variational method which treats the bosonic fields and the Klein factors on equal footing. As prototypical models we consider spinless fermions [1] and dimerized Hubbard chains [2].

[1] C. Mocanu, M. Dzierzawa, P. Schwab and U. Eckern, J. Phys.: Condens. Matter **16**, 6445 (2004).

[2] C. Mocanu, M. Dzierzawa, P. Schwab and U. Eckern, accepted for publication in Physica Status Solidi (b) (cond-mat/0411315).

TT 16.41 Sa 11:00 Poster TU C

Charge order in organic linear chain compounds investigated by ESR — •Belal Salameh, Michael Dumm , and Martin Dressel — 1.Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70555 Stuttgart.

We investigated the ferroelectric charge ordered state of the quasi one-dimensional organic charge-transfer salts $(TMTCF)_2X$ (C=Se, S; X=PF_6,AsF_6, SbF_6, BF_4 and SCN) by performing comprehensive ESR experiments in the temperature range from 4 to 300 K. At high temperatures, all investigated compounds show a linear decrease of the linewidth with decreasing temperature. Below T $\approx$ 200 K the linewidth starts to decrease more rapidly with lowering the temperature. We will discuss different models for this general behaviour of the ESR linewidth in the organic spin chain compounds investigated. For the sulfur salts the anisotropy and the temperature dependence of the ESR linewidth change below the charge ordering (CO) transition around 100 K. The characteristic changes of the angular dependence of the linewidth well below T_{CO} will be discussed in detail. Our findings in the charge ordered region might be due to the formation of two magnetically inequivalent TMTTF sites below the charge ordering transition temperature.

TT 16.42 Sa 11:00 Poster TU C

Optical spectroscopy of magnetic excitations — •E. Benckiser[1], M. Grüninger[1], T. Nunner[2], T. Kopp[2], C. Sekar[3], G. Krabbes[3], and A. Revcolevschi[4] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Experimentalphysik VI, Universität Augsburg — [3]IFW Dresden — [4]Laboratoire de Physico-Chimie de l'Etat Solides, Universite Paris-Sud, France

The magnetic excitations of several low-dimensional spin systems have been studied systematically by means of phonon-assisted infrared absorption. We present the optical conductivity $\sigma(\omega)$ of the 1D S=1/2 chain compound $SrCuO_2$, of the S=1/2 pseudo-ladder compound $CaCu_2O_3$ and of the 2D system $Ba_2Cu_3O_4Cl_2$. $CaCu_2O_3$ has been discussed as a two-leg S=1/2 ladder with $J_\perp \ll J_\parallel$. A detailed analysis of the optical conductivity shows that $CaCu_2O_3$ is rather a 3D system of weakly coupled chains with $J_\parallel \approx 165$ meV, where the two couplings perpendicular to the chains are much weaker but comparable with each other. The compound $SrCuO_2$ contains antiferromagnetic double-chains with J ≈ 181 meV, whereas the inter-chain coupling is weak ferromagnetic and frustrated. The 2D Cu_3O_4 layers in $Ba_2Cu_3O_4Cl_2$ contain a CuO_2 square lattice plus a second Cu square lattice with a much weaker coupling constant J_2. For $\omega \gg J_2$ the compound represents a clean realization of an undoped CuO_2 layer. We find that the high-energy spectral weight above the 2-magnon peak is larger than assumed previously.

TT 16.43 Sa 11:00 Poster TU C

Interchain Coupling in Mixed-Spin Quantum-Ferrimagnets — •Simon Grossjohann, Andreas Honecker, and Wolfram Brenig — Institut für Theoretische Physik, Technische Universität Braunschweig, Germany

We present an analysis of the thermodynamic properties of 1D- and 2D-mixed-spin quantum-magnets. Using the *Stochastic Series Expansion* method for evaluating the partition function we provide results for the uniform susceptibility and the static structure factor. The relevance of the *Random Phase Approximation* to describe interchain-exchange is investigated by extracting effective interchain-coupling-constants from our numerical findings. Furthermore, we provide a finite-size-scaling analysis of the static structure factor for selected system-parameters to adress the question of zero temperature long-range magnetic ordering. Finally we comment on the relation of our results to bulk thermodynamic data recently observed in the molecular ferrimagnet $MnNi(NO_2)_4(en)_2$.

TT 16.44 Sa 11:00 Poster TU C

Interplay between structure, magnetism and ordering phenomena in $La_{2-x}Sr_xCoO_4$ — •M. Cwik[1], M. Benomar[1], M. Haider[1], T. Lorenz[1], Y. Sidis[2], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Laboratoire Léon Brillouin, C.E.A./C.N.R.S., France

La_2CoO_4 is an antiferromagnetic insulator with $T_N \sim 275$ K and Co^{2+} in the S=3/2 high-spin state [1]. Doping with Sr induces a Co^{2+}/Co^{3+} mixed valency, destroys long-range antiferromagnetic order and removes the concomitant orthorhombic distortion of the K_2NiF_4 structure. In the half-doped compound $La_{1.5}Sr_{0.5}CoO_4$ spin and charge order have been found [2,3]. However, the effective magnetic coupling and the role of the three possible Co^{3+} spin states are not yet clarified. So far, it is also unknown how variations of doping affect both types of order in the $La_{2-x}Sr_xCoO_4$ series. We present a study of structure, spin order, charge order, magnetic fluctuations, resistivity, and susceptibility on high-quality single crystals for 0.2≤x≤1.0. We find a drastic change in the tetragonal CoO_6-octahedra distortion which is not consistent with a simple ionic picture and incommensurable spin order next to the half-doped compound. An analysis of the magnon dispersion suggests an effective three-dimensional magnetic coupling scheme away from a simple frustrated antiferromagnetic square lattice with competing nearest- and next-nearest-neighbor interaction.

[1] K. Yamada *et al.*, Phys. Rev. B **39**, 2236 (1989)
[2] I. A. Zaliznyak *et al.*, Phys. Rev. Lett. **85**, 4353 (2000)
[3] I. A. Zaliznyak *et al.*, Phys. Rev. B **64**, 195117 (2001)

TT 16.45 Sa 11:00 Poster TU C

Transport and Thermodynamic Properties of $RCoO_3$, R = La, Pr, Nd and Eu — •M. Kriener, K. Berggold, J. B aier, S. Jodlauk, H. Kierspel, T. Lorenz, M. Reuther, C. Zobel, and A. Freimuth — II. Physikalisches Institut, Universität zu Köln, 50937 Köln

$LaCoO_3$ is an insulator with unusual magnetic properties. Around 100 K $LaCoO_3$ shows a temperature-induced spin-state transition from a nonmagnetic low-spin state (electronic configuration of the Co^{3+}-ions: $t_{2g}^6e_g^0$ with $S=0$) to an intermediate-spin state ($t_{2g}^5e_g^1$ with $S=1$) [1]. Around 500 K a metal-insulator transition occurs. The spin state of Co^{3+} is determined by the balance of crystal-field splitting and Hund's rule coupling. We have studied the influence of an enhanced crystal field by substituting the La^{3+} ions by smaller isovalent rare-earth ions. Our study of the magnetic susceptibility, the thermal expansion and the electrical resistivity shows that Eu-doping causes a strong shift of the spin-state transition to higher temperatures, whereas the metal-insulator transition temperature increases only moderately [2]. Moreover, at low temperatures the thermal conductivity is strongly suppressed due to the spin-state transition in $LaCoO_3$. Replacing La completely by R = Pr, Nd or Eu systematically increases the thermal conductivity with decreasing radius of R, because of the shift of the spin-state transition towards higher temperatures.

[1] C. Zobel *et al.*, Phys. Rev. B **66**, 020402(R) (2002)
[2] J. Baier *et al.*, appears in Phys. Rev. B, cond-mat 0405680 (2004)
Supported by the DFG through SFB 608.

TT 16.46 Sa 11:00 Poster TU C

The optical properties of charge ordered Fe_3O_4 — •Alexander Yaresko[1,2], Ivan Leonov[3,4], Victor Antonov[2], Michail Korotin[4], and Vladimir Anisimov[4] — [1]MPI PKS, Noethintzer Str. 38, 01187, Dresden, Germany — [2]Institute of Metal Physics, Kiev, Ukraine — [3]Theoretical Physics III, Instituite for Physics, University of Augsburg, Germany — [4]Institute of Metal Physics, Russian Academy of Science-Ural Division, Yekaterinburg, Russia

Charge and orbital ordering in the low-temperature monoclinic phase of magnetite (Fe_3O_4) and its optical and magneto-optical properties are investigated using the LSDA and LSDA+U approaches. It is found that while the difference between t_{2g} minority occupancies of Fe_B^{2+} and Fe_B^{3+} cations is large and gives direct evidence for charge ordering, the screening is so effective that the total 3d charge disproportion is rather small. The calculated optical spectra agree well with the experimental ones. A band-by-band decomposition of the calculated optical conductivity allows to relate the experimentally observed peaks to particular interband transitions.

TT 16.47 Sa 11:00 Poster TU C

Electrostatically driven charge ordering in Fe_2OBO_3 — •I. Leonov[1], A. N. Yaresko[2], V. N. Antonov[3], and V. I. Anisimov[4] — [1]Theoretical Physics III, Institute for Physics, University of Augsburg — [2]Max-Planck Institute for the Physics of Complex Systems, Dresden — [3]Institute of Metal Physics, Vernadskii Street, 03142 Kiev, Ukraine — [4]Institute of Metal Physics, Russian Academy of Science-Ural Division, 620219 Yekaterinburg GSP-170, Russia

Charge ordering in the low-temperature monoclinic structure of iron oxoborate (Fe_2OBO_3) is investigated using the local spin density approximation with Coulomb interaction correction (LSDA+U) method. While the difference between t_{2g} minority occupancies of Fe^{2+} and Fe^{3+} cations is large and gives direct evidence for charge ordering, the screening is so effective that the total 3d charge disproportion is rather small. The occupied Fe^{2+} and Fe^{3+} cations are ordered alternately within the chain which is infinite along a-direction, resulting in ferromagnetic intrachain order due to $d^5 - d^6$ superexchange. The charge order obtained by LSDA+U is consistent with observed enlargement of the β angle.

TT 16.48 Sa 11:00 Poster TU C

High-Energy Scattering Study of Charge and Orbital Order of $Pr_{0.7}(Ca_{0.9}Sr_{0.1})_{0.3}MnO_3$ under pressure — •S. Kiele[1], J. Geck[1], M. von Zimmermann[2], N. Wizent[1], B. Büchner[1], and M.M. Abd-Elmeguid[3] — [1]Institut für Festkörperforschung, IFW Dresden, Helmholtzstr. 20, D-01171 Dresden — [2]Hamburger Synchrotronsstrahlungslabor am DESY, Notkestr. 85, D-22603 Hamburg — [3]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln

We present a high-energy scattering study of the superlattice reflections attributed to charge and orbital order in $Pr_{0.7}(Ca_{0.9}Sr_{0.1})_{0.3}MnO_3$ under hydrostatic pressure. Pure $Pr_{0.7}Ca_{0.3}MnO_3$ shows an antiferromagnetic insulating ground state with a longe-range charge and orbital order. Utilizing pressure it can be driven to a ferromagnetic metallic state, where the long-range charge order is destroyed. The Sr-substituted system can be understood in a phase separation scenario. Due to the different cation sizes, the double-exchange at the Sr-substituted sites changes, leading to

the formation of ferromagnetic metallic non-charge ordered regions in the antiferromagnetic insulating charge ordered background. Under external pressure we found a drastic decrease of the onset of the charge/orbital ordering temperature and a thermal hysteresis of the order parameter. The measurements have been done at the HASYLAB beamline BW5 with a three-crystal setting utilizing a new implementation of a clamp-type piston-cylinder cell of a relatively small size and reduced wall thickness in a closed-cycle cryostat on a four-circle diffractometer.

TT 16.49 Sa 11:00 Poster TU C

Low temperature behaviour of Sr and Ca doped manganites — •E. Forzani, V. Moshnyaga, and K. Winzer — I. Physikalisches Institut Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Perovskite manganites show insulator (I) to metal (M) phase transition, accompanied with a long range ferromagnetic ordering for doping level $x \geq 0.175$. Recently it was argued [1] that electronic phase separation of IM-type can take place due to the competition of double- and superexchange interactions even for chemically homogeneous samples. To check for the possible phase separation and thus recovering of insulating behaviour ($d\rho/d\,\mathrm{T} \leq 0$) at very low temperatures in the metallic samples, we studied single crystals and epitaxial films of Sr- and Ca-doped manganites. Measurements were carried out in a demagnetization cryostat for temperatures down to 40 mK and magnetic fields B = 0-7 T. As starting point, a $La_{1-x}Sr_xMnO_3$ ($x = 0.2$) single crystal exhibits metallic behaviour of the resistivity ρ(T) for 4.2 K $\leq$ T $\leq$ 300 K. The high residual resistivity ratio RRR = 58 and temperature coefficient of resistivity TCR $= 1/\rho(d\rho/d\mathrm{T}) \approx 13\%$/K by the IM-transition at 305 K confirm the high crystal quality.

Göttingen Graduate School of Physics and DFG (SFB 602, TP A2) are acknowledged.

[1] E.Dagotto, T.Hotta, A.Moreo, Physics Reports 344,1 (2001)

TT 16.50 Sa 11:00 Poster TU C

The electronic structure of $La_{1-x}Sr_xTiO_{3+\delta}$ — •Alexander Gössling, Reinhard Rückamp, Holger Roth, Thomas Lorenz, and Markus Grüninger — II. Physikalisches Institut, Universität zu Köln

Transition-metal oxides with orbital degeneracy have attracted a lot of interest. Their optical conductivity shows multi-peak structures in the visible und ultraviolet energy range. These excitations have been attributed to interband transitions either into the upper Hubbard band or the charge-transfer band. The spectral weight of the transitions from the lower into the upper Hubbard band sensitively depends on orbital and magnetic correlations. In this way, the physics of high ($\sim$ eV) and low ($\sim$ meV) energies is intimately connected.

In this context we studied the effect of hole doping on the optical conductivity of the Mott-Hubbard insulator $LaTiO_3$ in the range of 0.7 to 6.4 eV across the metal-insulator transition by means of ellipsometry. Furthermore we compare the spectra with the data of $YTiO_3$, having a reduced bandwidth. *Supported by the DFG through SFB 608.*

TT 16.51 Sa 11:00 Poster TU C

Comparison of X-ray absorption spectra of V_2O_3 at the O K edge to full multiple scattering calculations — •P. Pfalzer, J.-P. Urbach, J. Moosburger-Will, A. Nateprov, jr., M. Klemm und S. Horn — Universität Augsburg, Lehrstuhl für Experimentalphysik II, Universitätsstr. 1, 86135 Augsburg

X-ray absorption measurements at the O K edge are compared to full multiple scattering (FMS) calculations for the paramagnetic metallic, paramagnetic insulating and antiferromagnetic insulating phases of V_2O_3. The description of angular dependencies in experimentally recorded X-ray absorption near edge structure (XANES), even over an extended energy range, is possible with these calculations for the first time. Additionally, comparison of the experimental XANES with the FMS calculations corroborates the findings from EXAFS measurements, that V_2O_3 does not have local structure with trigonal symmetry in the metallic phase at room temperature. The observed large anisotropy of the XANES in the insulating phases is shown to be a direct consequence of the distorted physical structure. The calculations also suggest that the low energy part of the O 1s absorption edge is not rigorously split into a "t_{2g}"- and an "e_g"-part as suggested from bandstructure calculations.

TT 16.52 Sa 11:00 Poster TU C

Magnetic structure of $DyBaCo_2O_{5.5}$ — •H. Luetkens[1], H.-H. Klauss[2], A. Bosse[2], D. Cheptiakov[3], S. Streule[3], E. Pomjakushina[3], A. Podlesnyak[3], K. Conder[3], and P. Lemmens[4] — [1]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut CH-5232 Villigen PSI, Switzerland — [2]IMNF, TU Braunschweig, D-38106 Braunschweig, Germany — [3]Laboratory for Neutron Scattering ETHZ & PSI, CH-5233 Villigen PSI, Switzerland — [4]IHO, TU Braunschweig, D-38106 Braunschweig, Germany

The magnetic perovskite $REBaCo_2O_{5.5}$ system shows a rich magnetic and electronic phase diagram, with a MI transition at higher temperatures and magnetic ordering just below room temperature. Here, we report on neutron diffraction and muon spin rotation (μSR) measurements on a powder of $DyBaCo_2O_{5.5}$. From the neutron diffraction measurements an AFM (G-type) phase below 285 K is indicated by a doubling of the magnetic unit cell along both the crystallographic a and c axis. Further cooling below 260 K leads to a second magnetic phase which can be equally well described by two different spin-state ordered AFM structures. Microscopically, three magnetic transitions at 285 K, 260 K and 162 K have been observed by μSR. The high as well as the low temperature phase both show well defined muon spin precession characteristic for long range magnetic order. In the high temperature regime it was possible to independently measure the magnetic order parameter as well as the magnetic volume fraction. Additionally, at low temperatures a slowing down of the fluctuating Dy moment is observed by a characteristic peak in the longitudinal relaxation rate.

TT 16.53 Sa 11:00 Poster TU C

A Raman study of the charge-density-wave system $A_{0.3}MoO_3$ (A=K,Rb) — •D. M. Sagar[1], D. Fausti[1], P. H. M. van Loosdrecht[1], S. Yue[2], C. A. Kuntscher[2], M. Dressel[2], and S. van Smaalen[3] — [1]Material Science Center, University of Groningen, 9747 AG Groningen, The Netherlands — [2]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [3]Laboratory of Crystallography, University of Bayreuth, 95440 Bayreuth, Germany

The Peierls instability in (quasi-)one-dimensional metals leads to the formation of a charge-density-wave ground state at reduced temperatures. The fundamental excitations of this state, phasons and amplitudons, are strongly coupled charge-lattice excitations. While the infrared-active pinned phason mode is relatively well studied by various spectroscopic techniques, less is known on the low frequency Raman-active amplitudons. We present results of a Raman study of the well known bronzes $A_{0.3}MoO_3$ (A = K,Rb), focusing not only on the amplitudon mode but also on the so-called phase phonons in the charge-density-wave state, as well as on the observed pre-transitional Peierls fluctuations in the high temperature phase. *Supported by the NWO, DN-67-310, and DFG, SPP 1073.*

TT 16.54 Sa 11:00 Poster TU C

Doping effects on the electrical properties of blue bronze $K_{0.3}MoO_3$ — •S Yue[1], C. A Kuntscher[1], M Dressel[1], S van Smaalen[2], F Ritter[3], and W Assmus[3] — [1]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Laboratory of Crystallography, University of Bayreuth, 95440 Bayreuth, Germany — [3]Physikalisches Institut, Universität Frankfurt, 60054 Frankfurt, Germany

The temperature dependence of the dc resistivity and the nonlinear transport properties in pure, rubidium-, and tungsten-doped blue bronze $K_{0.3}MoO_3$ single crystals are presented. In comparison with the rubidium doping, the tungsten doping has larger effects on the electrical transport properties and the Peierls transition. In particular, the peak in the threshold field for nonlinear transport, observed in the pure and rubidium-doped samples around 100 K, is absent in tungsten-doped $K_{0.3}MoO_3$. These results are discussed with respect to the proposed incommensurate-commensurate transition of the charge-density-wave and its interaction with impurities. *Supported by the DFG, SPP 1073.*

TT 16.55 Sa 11:00 Poster TU C

Doping and pressure dependence of the optical properties of quasi-one-dimensional $LaTiO_{3.4}$ — •C. A. Kuntscher[1], K. Thirunavukkuarasu[1], S. Frank[1], I. Loa[2], K. Syassen[2], and F. Lichtenberg[3] — [1]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — [3]Experimentalphysik VI, EKM, Universität Augsburg, 86135 Augsburg, Germany

The perovskite-related compound $LaTiO_{3.4}$ shows a quasi-one-dimensional metallic character, which can be explained by its crystal structure consisting of chains of TiO_6 octahedra [1,2]. Based on temperature-dependent optical studies, a conduction mechanism involving polaronic quasiparticles was recently suggested [2]. To clarify the importance of polarons in $LaTiO_{3.4}$ polarization-dependent infrared reflectivity measurements were carried out as a function of doping and pressure. Besides the conduction mechanism, the issues of pressure-induced dimensional crossover and pressure dependence of phonon modes will be discussed. *Supported by the DFG, Emmy Noether-program.*

[1] F. Lichtenberg et al., *Prog. Solid State Chem.* **29**, 1 (2001).
[2] C. A. Kuntscher et al., *Phys. Rev. B* **67**, 035105 (2003).

TT 16.56 Sa 11:00 Poster TU C

Electronic and vibrational properties of low-dimensional perovskite-related $(Sr,La)NbO_{3.5-x}$ — •C. A. Kuntscher[1], P. Haas[1], B. Gorshunov[1,2], M. Dressel[1], and F. Lichtenberg[3] — [1]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [2]General Physics Institute, Russian Academy of Sciences, Moscow, Russia — [3]Experimentalphysik VI, EKM, Universität Augsburg, 86135 Augsburg, Germany

Polarization-dependent infrared reflectivity measurements on various $(Sr,La)NbO_{3.50-x}$ single crystals [1] were carried out as a function of temperature [2]. All compounds have highly anisotropic optical properties; in particular, $SrNbO_{3.41}$ and $SrNbO_{3.45}$ show a Drude-like behavior along the chain direction and a semiconducting behavior along the perpendicular direction. In contrast, for $Sr_{0.8}La_{0.2}NbO_{3.50}$ the Drude contribution is very small, and has vanished completely for the ferroelectric insulator $SrNbO_{3.50}$. With decreasing temperature, for $SrNbO_{3.41}$ and $SrNbO_{3.45}$ a suppression of spectral weight is observed in the low-frequency optical conductivity for $\mathbf{E}\|a$, with the development of a pronounced peak, which can be interpreted in terms of the opening of an energy gap of only a few meV. The gap opening most probably is due to a Peierls-type instability. In contrast, no energy gap is found for $Sr_{0.8}La_{0.2}NbO_{3.50}$, which can be related to differences in the crystal structure. *Supported by the DFG.*

[1] F. Lichtenberg et al., *Prog. Solid State Chem.* **29**, 1 (2001).
[2] C. A. Kuntscher *et al.*, to appear in Phys. Rev. B (2004).

TT 16.57 Sa 11:00 Poster TU C

Optical and magnetic properties of low-dimensional perovskite-related $(La,Ca)TiO_{3.4\pm\delta}$ — •K. Thirunavukkuarasu[1], F. Lichtenberg[2], and C. A. Kuntscher[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Experimentalphysik VI, EKM, Universität Augsburg, 86135 Augsburg, Germany

The perovskite-related titanium oxides $LaTiO_{3.5-x}$ with $0 \leq x \leq 0.5$ show a rich phase diagram, including a Mott-Hubbard insulator with antiferromagnetic ordering (x=0.5), metallic phases, semiconductors, and a ferroelectric insulator (x=0) [1]. In particular, for $x \approx 0.1$ the dc resistivity is strongly anisotropic, with metal-like values along the a axis. The optical conductivity spectrum contains a Drude component only for the polarization $\mathbf{E}\|a$, indicating the quasi-one-dimensional metallic character of $LaTiO_{3.4}$ [2].

We carried out polarization-dependent infrared reflectivity measurements and magnetic susceptibility measurements on various $(La,Ca)TiO_{3.4\pm\delta}$ single crystals. For all studied crystals the optical conductivity along the chain direction a consists of a Drude-like contribution superimposed by phonon modes, and a pronounced band in the midinfrared range centered at 2000-3000 cm^{-1}($\approx$250-370 meV). For increasing carrier doping or decreasing temperature a shift of the midinfrared band towards lower frequencies is observed. These findings are discussed in terms of polaronic models.

[1] F. Lichtenberg et al., *Prog. Solid State Chem.* **29**, 1 (2001).
[2] C. A. Kuntscher et al., *Phys. Rev. B* **67**, 035105 (2003).

TT 16.58 Sa 11:00 Poster TU C

Ab-initio Phonons for the layered compound TiOCl — •Leonardo Pisani and Maria-Roser Valenti — Institute for Theoretical Physics, University of Frankfurt, 60054 Frankfurt, Germany

We present first-principles frozen-phonon calculations for the determination of the three Raman-active A_g modes in the spin-1/2 layered TiOCl system within two different well-known approaches: the generalized gradient approximation (GGA) and the so-called LDA+U approximation. We observe that the inclusion of electron correlation in a mean-field level as implemented in the LDA+U leads to a better overall agreement with experimental results. We also discuss the implications of the two approaches on the physics of TiOCl.

TT 16.59 Sa 11:00 Poster TU C

Quantenoszillationsexperimente an Θ-$(BEDT\text{-}TTF)_2I_3$ — •Axel Nothardt[1], Edurart Balthes[1], Belal Salameh[1], Wolfgang Schmidt[1], Dieter Schweitzer[1] und Duncan Maude[2] — [1]3. Physikalisches Instiut, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart — [2]MPI/CNRS Hochmagnetfeldlabor Grenoble, Avenue des Martyrs 25, B.P. 166, F-38042 Grenoble Cedex 9, Frankreich

Es ist erstmals gelungen durch ausschließliches Verwenden von I_3^{-1} Anionen den organischen Supraleiter Θ-$(BEDT\text{-}TTF)_2I_3$ (BEDT-TTF = Bisethylendithiotetrathiofulvalen) als reine Einkristalle auf elektrochemische Weise zu synthetisieren (T_C=3.6K). Die Fermifläche wurde winkelabhängig mit Quantenoszillationsmessungen, sowohl in Magnetisierung (dHvA) als auch in Leitfähigkeit (SdH), untersucht. Die Wellung der Fermifläche, die wegen der Quasi-Zweidimensionalität des elektronischen Systems nahezu ein Zylinder ist, konnte mit den Schwebungsfrequenzen für das α-Orbit (F_α=780T) und das β-Orbit (F_β=4200T) mit ΔF_α=6.5T und ΔF_β=16T bestimmt werden. Die Schwebungsknoten von F_β liegen an denen von Yamaji berechneten Positionen. Die Knoten von F_α liegen hingegen deutlich verschoben zu den erwarteten Positionen. Mit diesen Knotenverschiebungen, die ertsmals an β-$(BEDT\text{-}TTF)_2IBr_2$ und an $(BEDT\text{-}TTF)_4[Ni(dto)_2]$ entdeckt wurden, können neueste Theorien bezüglich der Knotenverschiebung verifiziert werden. Die Größe eines weiteren Orbits, das dreidimensional ist, wurde winkelabhängig untersucht, wobei die zugehörigen Oszillationsfrequenzen von $F_\gamma(90°)$=1,8T bis $F_\gamma(0°)$=7,8T reichen.

TT 16.60 Sa 11:00 Poster TU C

Untersuchungen von Schwebungsknoten bei Quantenoszillationsmessungen (dHvA und SdH) am $(BEDT\text{-}TTF)_4[Ni(dto)_2]$ — •Wolfgang Schmidt, Axel Nothardt, Eduard Balthes und Dieter Schweitzer — 3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Mit Quantenoszillationsexperimenten sowohl in Leitfähigkeit (SdH) als auch in Magnetisierung (dHvA) wurde bei der Fermifläche von $(BEDT\text{-}TTF)_4[Ni(dto)_2]$ das α-Orbit ($F_\alpha = 634$T) und das β-Orbit ($F_\beta = 4245$T) gefunden. Aufgrund der gewellten Fermifläche sind die Oszillationen mit einer Schwebung überlagert. Yamaji berechnete hierzu die Positionen der Schwebungsknoten. Überraschenderweise weichen die Knotenpositionen bei SdH-Messungen deutlich von diesen Berechnungen ab. Diese Verschiebung wurde in den organischen Metallen $(BEDT\text{-}TTF)_4[Ni(dto)_2]$ [1] und β-$(BEDT\text{-}TTF)_2IBr_2$ [2] untersucht, die beide mehrere Schwebungsknoten zeigen. Mehrere Knoten sind nötig, um die Theorie von Yamaji und aktuell diskutierte Theorien über die Ursache der Phasenverschiebung der Schwebung zu verifizieren [3].

Hier werden winkelabhängige Messungen von bis zu vier Schwebungsknoten erörtert und mit den Theorien verglichen.

[1] M. Schiller et al.: Europhys. Lett. 51, 82 (2000)
[2] M.V. Kartsovnik et al.: Phys. Rev. Lett. 89, 126802 (2002)
[3] P.D. Grigoriev: Phys. Rev. B 67, 144401 (2003)

TT 16.61 Sa 11:00 Poster TU C

Electron Spin Resonance and Transport Measurements on the neat Organic Superconductor Θ-$(BEDT\text{-}TTF)_2I_3$ — •Belal Salameh, Axel Nothardt, Anja Much, and Dieter Schweitzer — 3.Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

On crystals of the neat organic superconductor Θ-$(BEDT\text{-}TTF)_2I_3$ transport and magnetic properties have been investigated by means of ESR, SQUID and dc measurements. From the dc resistivity and susceptibility measurements this material has a typical metallic behaviour from room temperature down to the superconducting transition temperature

($T_c = 3.6$ K). The room temperature resistivities parallel and perpendicular to the conduction plane are typically 0.04 and 20 Ω·cm respectively. The resistivities decrease about three orders of magnitude at 4.2 K. The ESR linewidth ranges from about 60 to 80 G at room temperature and decreases with decreasing temperature down to about 8 G at 20 K. Below 20 K the linewidth increases again slightly probably due to magnetic interactions. At room temperature our crystals exhibit Dysonian line shape when the microwave magnetic field is applied perpendicular to the conduction plane and a Lorentzian lineshape when the microwave magnetic field is parallel to the conduction plane. The Lorentzian line is gradually converted to a Dysonian shape with decreasing temperature below about 250 K due to a significant decrease in the skin depth.

TT 16.62 Sa 11:00 Poster TU C

Pressure-induced dimensional crossover in the quasi-one-dimensional Mott-Hubbard insulator $(TMTTF)_2AsF_6$ — •A. Pashkin, M. Dressel, and C. A. Kuntscher — 1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

The organic $(TMTTF)_2X$ salts consist of basically uncoupled molecular stacks (half-filled) and are prime examples of one-dimensional Mott-Hubbard insulators. With increasing interchain hopping the systems become more metallic, as can be realized in the metallic TMTSF analogs where the coupling between the chains is enhanced. This dimensional crossover can be best explored experimentally by tuning of the interstack interaction with external pressure. A complete theoretical description is still missing for the case of a strictly one-dimensional half-filled chain when going to a more two-dimensional system.

We have studied the pressure dependence (<10 GPa) of the reflectivity of $(TMTTF)_2AsF_6$ along the molecular stacking axis a and along the b-direction. The evolution of the reflectivity with increasing pressure demonstrates the gradual onset of a Drude-like conductivity along b'. At high enough pressure (>3 GPa) the infrared response along both directions becomes similar to that of the conducting TMTSF-analogs in accordance with the generalized temperature-pressure phase diagram. We also discuss the behavior of the phonon modes with change of the pressure.

TT 16.63 Sa 11:00 Poster TU C

Dynamic phonons and charge order in a quarter-filled ladder — •T. C. Lang, D. R. Neuber, M. Aichhorn, and H. G. Evertz — Institute for Theoretical and Computational Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria

We investigate the charge order transition of a quarter-filled extended Hubbard-Holstein ladder at finite temperature as a model for sodium vanadate. Based on the canonical Lang-Firsov transformation of the Hamiltonian, a principle component representation of the phonon degrees of freedom allows us to sample phonon configurations in the framework of determinantal Quantum Monte Carlo much more efficiently than previously possible. The sign problem is moderate in a wide range of model parameters relevant for α'-NaV_2O_5. Experiments and previous calculations imply great relevance of the lattice coupling to the charge order transition. Low frequency lattice vibrations increase the charge order, accompanied by dynamically produced zig-zag lattice distortions. The single-particle spectral function, spin- and charge-spectra of the ladder in the presence/absence of dynamic phonons are obtained.

TT 16.64 Sa 11:00 Poster TU C

Spin gap and charge order in weakly coupled quarter-filled ladders — •Bernhard Edegger[1,2], Hans Gerd Evertz[2], and Reinhard M. Noack[3] — [1]Theoretische Physik, Universität des Saarlandes — [2]Insitut für Theoretische Physik, Technische Universität Graz — [3]Fachbereich Physik, Philipps Universität Marburg

We present DMRG (Density Matrix Renormalization Group) calculations in quarter-filled ladders with model parameters relevant for NaV_2O_5. The properties of the low temperature phase are well described by including the coupling of the electrons to static lattice distortions in the extended Hubbard model. Charge order, charge gap and the effective magnetic exchange constant are determined. In addition, we show that a spin gap is induced by super-anti-ferroelectric charge order in weakly coupled quarter-filled ladders.

TT 16.65 Sa 11:00 Poster TU C

Parent Hamiltonian for the SU(3) trimer chain — •Stephan Rachel, Dirk Schuricht, and Martin Greiter — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe (TH), Postfach 6980, D-76128 Karlsruhe

In analogy to the Majumdar–Gosh model, which describes a dimerized chain of SU(2) spins, we present a Hamiltonian for an SU(3) spin chain, the ground state of which consists of SU(3) singlets of triples of neighboring spins. This Hamiltonian is local, translationally invariant, and consists only of two-spin interactions. We use the model to show that the fractionally quantized elementary excitations of the SU(3) trimer chain, the colorons, transform under representation $\bar{3}$ under SU(3) transformations if the spins of the original model transform under representation 3. In other words, if a basis for the spins on the chain is spanned by the colors blue, red, and green, a basis for the coloron excitations is given by the complementary colors yellow, cyan, or magenta.

TT 16.66 Sa 11:00 Poster TU C

Microscopic theory of half-metallic double perovskites — •Nils Blümer, Carsten Knecht, Krunoslav Požgajčić und P. G. J. van Dongen — Institut für Physik, Johannes Gutenberg - Universität, 55099 Mainz

Half-metallic double perovkites such as Sr_2FeReO_6 and Sr_2FeReO_6 are promising materials for spintronic applications. Due to the strong correlations associated with the Fe sites, conventional band structure calculations are not reliable for this class of systems. We review the present status of correlated-electron approaches for double perovskite materials and outline our strategy for microscopic calculations using an improved algorithm for quantum Monte Carlo simulations within the framework of dynamical mean-field theory (DMFT). Prospects for application of the recently developed self-energy functional theory in this context are also discussed. Funded by DFG: FOR 559/1.

TT 16.67 Sa 11:00 Poster TU C

Itinerant electron metamagnetism and weak ferromagnetism in $LaCo_9Si_4$ and YCo_9Si_4 — •H. Michor[1], S. Özcan[1], M. El-Hagary[1], E. Bauer[1], M. Reissner[1], G. Hilscher[1], S. Khmelevskyi[2], P. Mohn[2], P. Rogl[3], and H. Rosner[4] — [1]Institut für Festkörperphysik, T.U. Wien, A-1040 Wien, Austria — [2]Center for Computational Materials Science, T.U. Wien, Austria — [3]Institut für Physikalische Chemie, Universität Wien, Austria — [4]Max-Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany

$LaCo_9Si_4$ is a strongly exchange enhanced Pauli paramagnet with an instability towards weak ferromagnetism, i.e. exhibits itinerant electron metamagnetism at about 3.5 T for $H||c$ and 6 T for $H\perp c$, which is the lowest value ever found for rare earth intermetallic compounds [1]. Despite of the smaller unit cell volume isostructural and isoelectronic YCo_9Si_4 exhibits a weak itinerant ferromagnetic ground state ($T_C \simeq 25$ K) already in zero-field. The ground state properties of La- and YCo_9Si_4 are discussed on basis of magnetisation, specific heat, and resistivity measurements and via ab-initio electronic structure calculations. The band structure calculations result in a ferromagnetic groundstate for both compounds with moments substantialy larger than the experimentally observed moments. The origin of these discrepancies is briefly discussed. [1] H. Michor et al., Phys.Rev. B **69** (2004) 081404(R).

TT 16.68 Sa 11:00 Poster TU C

Magnetic Ordering in Trigonal Chain Compounds — •Christian Laschinger[1], Udo Schwingenschlögl[1], Volker Eyert[1], Thilo Kopp[1], Raymond Frésard[2], and Ulrich Eckern[1] — [1]University of Augsburg — [2]Institut des Sciences de la Matière et du Rayonnement, Caen, France

We investigate the microscopic origin of the ferromagnetic and antiferromagnetic spin exchange couplings in the quasi-one-dimensional cobalt compounds Ca_3ABO_6 with A = Fe, Co and B = Co, Rh. From electronic structure calculations we find A 3d low spin and high spin states alternating along the characteristic chains. In addition strong d-p hybridisation leads to the formation of extended localized magnetic moments centered at the high spin sites. Antiferromagnetic coupling along the chains is induced by a strong metal-metal overlap via the $d_{3z^2-r^2}$ orbitals of the low spin sites. It competes with ferromagnetic exchange, which originates in a cyclic exchange through the ligand atoms.

TT 16.69 Sa 11:00 Poster TU C

Dimerization pattern or two-dimensional spin systems with spin phonon coupling in the adiabatic limit — •Carsten Aits[1], Ute Löw[1], and Andreas Klümper[2] — [1]Universität zu Köln, Institut für Theoretische Physik, Zülpicher Str.77, D-50937 Köln — [2]Bergische Universität Wuppertal, Theoretische Physik, D-42097 Wuppertal

Little is known about the ground state phase diagram of two-dimensional spin systems with spin phonon coupling. In the adiabatic limit, however, they correspond to spin models with inhomogeneous couplings. In contrast to the one-dimensional case, where the dimerization pattern is unique, it is not clear how the two-dimensional lattice responds to a non-vanishing spin phonon coupling. As far as the S=1/2 Heisenberg model is concerned, different choices of inhomogenous patterns of couplings lead to rather different ground state properties with magnetic energy gain that may or may not compete with the energy loss of the phonon system.

We apply a loop algorithm in continuous Trotter time to clarify which distortion pattern is energetically favored. Our approach is twofold. First, we extrapolate the ground state energies and magnetizations for various patterns of alternating couplings and analyze whether a transition to a gapped state appears. Second, we consider an expansion of the free energy of the distorted models at the point of vanishing distortion. In the adiabatic limit, this corresponds to an analysis of spin layers coupled to three dimensional phonons at finite temperatures. We determine the coefficients of the leading order from the (Euclidean) dynamical dimer correlation functions, which are directly accessible within our method.

TT 16.70 Sa 11:00 Poster TU C

Incommensurate spin dynamics in underdoped cuprate perovskites — •Alexei Sherman[1] and Michael Schreiber[2] — [1]Institute of Physics, University of Tartu, Estonia — [2]Institut für Physik, Technische Universität Chemnitz

The incommensurate magnetic response observed in normal-state cuprate perovskites is interpreted based on the memory function formalism and the t-J model of Cu-O planes. In agreement with experiment the calculated dispersion of maxima in the susceptibility has the shape of two parabolas with upward and downward branches which converge at the antiferromagnetic wave vector. The maxima are located at the momenta $(\frac{1}{2}, \frac{1}{2} \pm \delta)$, $(\frac{1}{2} \pm \delta, \frac{1}{2})$ and at $(\frac{1}{2} \pm \delta, \frac{1}{2} \pm \delta)$, $(\frac{1}{2} \pm \delta, \frac{1}{2} \mp \delta)$ in the lower and upper parabolas, respectively. The upper parabola reflects the dispersion of magnetic excitations of the localized Cu spins, while the lower parabola arises due to a dip in the spin-excitation damping at the antiferromagnetic wave vector. For moderate doping this dip stems from the weakness of the interaction between the spin excitations and holes near the hot spots. The frequency dependence of the susceptibility is shown to depend strongly on the hole bandwidth and damping and varies from the shape observed in $YBa_2Cu_3O_{7-y}$ to that inherent in $La_{2-x}Sr_xCuO_4$.

TT 16.71 Sa 11:00 Poster TU C

Structural properties of $RETiO_3$ and $Y_{1-x}Ca_xTiO_3$ — •A. Komarek[1], H. Roth[1], T. Lorenz[1], W.D. Stein[1], M. Cwik[1], F. Bourée[2], A. Freimuth[1], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Laboratoire Léon Brillouin

We have studied the crystal structure of the $RETiO_3$ by different diffraction techniques as function of temperature. In all compounds we find significant distortions of the TiO_6-octahedra which lead to a lifting of the t_{2g}-orbital degeneracy. A comparison with literature data on isostructural compounds with a $3d^0$ or a $4d^0$-configuration shows that such distortions not necessarily are caused by orbital physics. In the $RETiO_3$-series, however, the temperature dependence clearly points to a direct coupling. The octahedron distortions depend more sensitively on temperature than the tilt and rotation angles; and, in particular, we find strong anomalies at the Néel-temperatures in all antiferromagnetic $RETiO_3$ compounds.

Neutron diffraction on a sample of $Y_{0.62}Ca_{0.38}TiO_3$ yields strong evidence for charge ordering, which may be the key element to understand, why Ca-doped $YTiO_3$ stays non-metallic till rather high doping.

TT 16.72 Sa 11:00 Poster TU C

Orbital excitations in transition-metal compounds — •R. Rückamp[1], A. Gössling[1], M. Grüninger[1], H. Roth[1], A. Freimuth[1], L. Jongen[2], A. Möller[2], G. Meyer[2], T.T.M. Palstra[3], A. Nugroho[3], and S.-W. Cheong[4] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Anorganische Chemie, Universität zu Köln — [3]Materials Science Centre, University of Groningen — [4]Department of Physics & Astronomy, Rutgers University, New Jersey

In recent years orbital physics has attracted much interest since novel phenomena - such as an orbital liquid state or new elementary excitations in an orbitally ordered state - have been predicted. In order to observe these phenomena, one has to look for a system in which the orbital (electron-electron) coupling dominates over the coupling to the lattice (Jahn-Teller effect). We have studied orbital excitations in the optical conductivity spectra of several transition-metal compounds such as $RTiO_3$, RVO_3, TiOX or Y_2BaNiO_5 by measuring both transmittance and reflectance of single crystals. The energies of the orbital (d-d) transitions are compared with the results of a point-charge model including the hybridisation with the ligand ions. We find good agreement between experiment and theory, which suggests that the coupling to the lattice is dominant in the studied compounds.

TT 16.73 Sa 11:00 Poster TU C

Structural properties of $Ca_{2-x}Sr_xRuO_4$ — •O. Schumann[1], P. Steffens[1], R. Müller[1], G. Andre[2], P.G. Radaelli[3], P. Adelmann[4], S. Nakatsuji[5], Y. Maeno[5], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Laboratoire Léon Brillouin — [3]ISIS Facility, Rutherford Appleton Laboratory — [4]Forschungszentrum Karlsruhe, IFP — [5]Department of Physics, Kyoto University

We present our x-ray- and neutron diffraction work on $Ca_{2-x}Sr_xRuO_4$ which shows an astonishing rich phase diagram, even though the substitution of Sr^{2+} by Ca^{2+} is an isovalent one [1]. Pure Sr_2RuO_4 (x=2) exhibits no structural distortions. Upon Ca-doping a rotation of the RuO_6-octahedron sets in. This phase transition is strongly discontinuous, although a continuous one is allowed by symmetry. At rather higher Ca-content (x$\sim$0.2) a metamagnetic transition is observed. The temperature and magnetic field dependence of small structural changes are an indication of an electron transfer between in- and out-of-plane t_{2g}-orbitals. This transfer is driven by a van-Hove singularity in one of the concerned bands [2]. At even higher Ca-content the rotational distortion changes its stacking sequence. While for x>0.2 the octahedrons in neighboring layers rotate out of phase, for x<0.2 the rotation between neighboring layers is in-phase. This rather subtle change is in coincidence with a change of the ground state properties of the samples (metallic vs. af insulating).

[1] O.Friedt *et al.*, Phys. Rev. B **63** 174432 (2001)
[2] M.Kriener *et al.*, condmat/0408015

TT 16.74 Sa 11:00 Poster TU C

Magnetic Field Dependence of Thermodynamic Properties of $(Ca,Sr)_2RuO_4$ — •J. Baier[1], T. Zabel[1], M. Kriener[1], P. Steffens[1], O. Schumann[1], O. Heyer[1], T. Lorenz[1], A. Freimuth[1], O. Friedt[1], M. Braden[1], A. Revcolevschi[2], S. Nakatsuji[3], and Y. Maeno[3] — [1]II.Physikalisches Institut, Universität zu Köln, Germany — [2]Lab. de Physico-Chimie de l'État Solide, Université Paris-Sud, France — [3]Dep. of Physics, Kyoto University, Japan

We present a study of thermal expansion α and specific heat c_P of $Ca_{2-x}Sr_xRuO_4$ in magnetic fields. This series with the spin-triplet superconductor Sr_2RuO_4 and the antiferromagnetic Mott-insulator Ca_2RuO_4 as end members presents a rich spectrum of structural distortions accompanied by drastic changes of the magnetic and electronic properties [1]. We focus on $0.2 \leq x \leq 0.5$ where the compound is still metallic but close to localization. We find an anisotropic anomalous thermal expansion. The anomaly is suppressed by a magnetic field [2]. Below $T \simeq 20\,K$, α, c_P and the magnetization show an anisotropic field dependence. The $x = 0.2$ sample shows a metamagnetic transition (MMT) accompanied by a large magnetostriction. Furthermore, c_P/T shows a non-monotonic field dependence with a maximum at the MMT. For $x = 0.5$, c_p/T reaches an unusually large value in zero field and we observe a strong decrease of c_p/T in a magnetic field similar to the behavior of c_p/T at $x = 0.2$ above the MMT.

[1] Friedt *et al.*, Phys.Rev.B **63** (2001)
[2] Kriener *et al.*, cond-mat 0408015, submitted to Phys. Rev. Lett.
Supported by the DFG through SFB 608

TT 16.75 Sa 11:00 Poster TU C

Low temperature mixed spin state of Co^{3+} in $LaCoO_3$ evidenced from local lattice distortions — •V. Gnezdilov[1], P. Lemmens[2,3], Yu.G. Pashkevich[4], K.-Y. Choi[5], S. Shiry aev[6], G. Bychkov[6], and S. Barilo[6] — [1]B.I. Verkin Inst. for Low Temp. Physics NASU, 61164 Kharkov, Ukraine — [2]Inst. for Physics of Condensed Matter, TU Braunschweig, D-38106 Braunschweig, Germany — [3]MPI-FKF, D-70569 Stuttgart, Germany — [4]A.A. Galkin Donetsk Phystech NASU, 83114 Donetsk, Ukraine — [5]Inst. for Materials Research, Tohoku University, Sendai 980-8577, Japan — [6]Inst. of Physics of Solids & Semiconductors, Academy of Sciences, 220072 Minsk, Belarus

Single- and multi-phonon excitations of the single crystalline $LaCoO_3$ were studied using Raman spectroscopy in the temperature region of 5 K - 300 K. First-order Raman spectra show a larger number of phonon modes than allowed for the rhombohedral (D^6_{3d}) structure. Additional phonon modes are interpreted in terms of activated modes due to local lattice distortions arising from the Jahn-Teller (JT) activity of the intermediate-spin (IS) state of Co^{3+} ions. The temperature dependence of the breathing - and stretching-type phonon modes on cooling suggests the presence of Co^{3+} ions in the intermediate spin state, even at lowest temperatures. The anomalous temperature dependence of the second-order phonon excitations spectra is in accordance with the Franck-Condon mechanism that is characteristic for a JT orbital order.

TT 16.76 Sa 11:00 Poster TU C

Co^{3+} spin state transition detected by phonon Raman scattering in $GdBaCo_2O_{5.5}$ — •Yu.G. Pashkevich[1], V.P. Gnezdilov[2], P. Lemmens[3,4], B. Keimer[4], C. Ambrosch-D raxl[5], K.V. Lamonova[1], A.A. Gusev[1], K.-Y. Choi[6], S.N. Barilo[7], S.-V. Shiryaev[7], and G.-L. Bychkov[7] — [1]A.A. Galkin Donetsk Phystech NASU, 83114 Donetsk, Ukraine — [2]B.I. Verkin Inst. for Low Temp. Physics NASU, 61164 Kharkov, Ukraine — [3]Inst. for Physics of Condensed Matter, TU Braunschweig, D-38106 Braunschweig, Germany — [4]MPI-FKF, D-70569 Stuttgart, Germany — [5]Inst. für Theoretische Physik, Universität Graz, A-8010 Graz, Austria — [6]Inst. for Materials Research, Tohoku University, Sendai 980-8577, Japan — [7]Inst. of Physics of Solids & Semiconductors, Academy of Sciences, 220072 Minsk, Belarus

The change of the spin state of Co^{3+} as function of temperature or pressure is an intriguing feature of cobalt-based perovskite compounds. In the layered cobaltites $RBaCo_2O_5O_{5.5}$ this problem is rather complicated due to the octahedral and opened square pyramidal coordinations of Co with oxygen. Raman spectroscopy can provide information about subtle changes in spin state through detecting changes of the phonon spectra, which are sensitive to the O-Co-O bonding length and angles. Raman spectra of single crystal $GdBaCo_2O_5O_{5.5}$ were measured in the temperature range 5 - 400 K and remarkable changes of frequencies and intensities were observed. Frequencies and eigenvectors of Raman active phonon modes have been defined using frozen phonon ab initio band structure calculations and structural data at 300 K in Pmmm setting.

TT 16.77 Sa 11:00 Poster TU C

Finite Temperature Properties of the 2D Kondo-Necklace — •Wolfram Brenig — Institute for Theoretical Physics, Technical University of Braunschweig, Germany

We analyze several thermodynamic properties of the two-dimensional SU(2) Kondo-necklace. Using a quantum Monte-Carlo approach based on the stochastic series expansion method we provide results for the staggered structure factor as well as the uniform and staggered susceptibilities as a function of the temperature and 'Kondo'-exchange in the vicinity of the quantum critical point, which separates long-range antiferromagnetic order from dimerization in this system. We study the local susceptibility at criticality and find evidence for a power-law temperature dependence. Finally we investigate the crossover from classical to renormalized classical behavior via the quantum critical regime. Work supported in part by the DFG through SPP 1073.

TT 16.78 Sa 11:00 Poster TU C

Orbital ordering in manganites in the band approach. — •Dmitri Efremov[1] and Daniil Khomskii[2] — [1]TU Dresden, 01062 Dresden — [2]University of Cologne, 50937 Cologne

We consider the orbital ordering in $LaMnO_3$ and similar systems, proceeding from the band picture. For the realistic magnetic structure of A-type there exist the nesting between two e_g-bands and the nesting inside the bands. We show that the interband nesting is more effective. It results in an orbital ordering – orbital density wave (ODW), the type of which coincides with those existing in $LaMnO_3$.

TT 16.79 Sa 11:00 Poster TU C

Single hole dynamics across magnetic order-disorder quantum phase transitions. — •Christian Brünger and Fakher Assaad — Universität Würzburg

We consider a bi-layer Heisenberg model with interplanar (intraplanar) exchange $J_\perp$ (J). It is known that as a function of $J_\perp/J$ the model shows an order-disorder quantum phase transition. Our aim is to understand the behavior of the single particle spectral function of a doped hole in this magnetic background. In particular, the question of the vanishing of the quasiparticle weight in the vicinity of the quantum phase transition will be addressed. Our calculations are done within a self-consistent Born approximation as well as with the quantum Monte Carlo loop algorithm.

TT 16.80 Sa 11:00 Poster TU C

The Kimball-Overhauser approach to the pair density of the 3D electron gas and Friedel-like phase-shift sum rules — •Paul Ziesche — Max-Planck-Insitut fuer Physik komplexer Systeme, D-01187 Dresden

Kimball-Overhauser geminals follow from a 2-body Schroedinger equation with an appropriately screened Coulomb repulsion. They parametrize the pair density together with geminal occupancies, which follow from the non-idempotent momentum distribution [1]. The neutrality sum rule for the pair density leads to sum rules for the geminal phase shifts, which resemble the Friedel sum rule of solid-state physics [2]. Friedel-like oscillations originate from the singularities of the geminal weight [3]. [1] P. Gori-Giorgi and P. Ziesche, Phys. Rev. B 66, 235116 (2002) [2] P. Ziesche, Phys. Rev. B 67, 233102 (2003) [3] P. Ziesche, phys. stat. sol. (b), in press.

TT 16.81 Sa 11:00 Poster TU C

Quasiparticle bands of the ionic hubbard model — •Torben Jabben and Norbert Grewe — Institut für Festkörperphysik, Tu-Darmstadt,D-64289 Darmstadt

The ionic Hubbard model on a simple cubic lattice is investigated using analytical approximations and Wilson's renormalization group for the charge excitation spectrum near the Mott insulating regime. The corresponding partial spectral weights and local densities of states show characteristic features, which compare well with a hybridized-band picture appropriate for the regime at small U, which at half-filling is known as a band insulator. In particular, a narrow charge gap is obtained at half-filling in the ABR, and the distribution of spectral quasi-particle weight reflects the fundamental hybridization mechanism of the model.

TT 16.82 Sa 11:00 Poster TU C

Checkerboard Order in the projected $SO(5)$ model — •Martin Jöstingmeier[1], Stephan Hochkeppel[1], Werner Hanke[1], and Shou-Cheng Zang[2] — [1]Theoretische Physik, Am Hubland, D-97074 Würzburg, Germany — [2]Department of Physics, Stanford University, Stanford, 94305 California

Based on Contractor renormalization group calculations, it was recently proposed [1] to extend the projected $SO(5)$ model by offsite Coulomb repulsions. We study this model, using numerically essentially exact Quantum-Monte Carlo calculations, in order to clarify the ($T = 0$) phase diagram. We find antiferromagnetism, superconductivity as well different types of charge-ordered phases. In particular, we determine the type of the phase transition at a multicritical point, that is a possible candidate for $SO(5)$ symmetry restoration. Motivated by scanning tunneling microscopy experiments on $Bi_2Sr_2CaCu_2O_{8+\delta}$ and $Ca_{2-x}Na_xCuO_2Cl_2$ [2,3,4] , that observe charge ordering patterns, we also study in detail checkerboard order as function of doping as well as temperature.

[1] H.-D. Chen, S. Capponi, F. Alet, and S.-C. Zhang, Phys. Rev. B (2004).
[2] J. E. Hoffman, E. W. Hudson, K. M. Lang, V. Madhavan, H. Eisaki, S. Uchida, and J. C. Davis, Science **295**, 466 (2002).
[3] C. Howald, H. Eisaki, N. Kaneko, M. Greven, and A. Kapitulnik, Phys. Rev. B **67**, 014533 (2003).
[4] M. Vershinin, S. Misra, S. Ono, Y. Abe, Y. Ando, and A. Yazdani, Science **303**, 1995 (2004).

TT 16.83 Sa 11:00 Poster TU C

Generalization of Luttinger-Ward Functional and the Extended Variational Cluster Approach — •Ninghua Tong[1] and Ralf Bulla[2] — [1]Institute for Theory of Condensed Matter, University of Karlsruhe — [2]Theoretical Physics III, Institute for Physics, University of Augsburg

The Luttinger-Ward functional is generalized to a functional of more than one variable. Our generalization is based on the Legendre transformation to the grand potential functional, and therefore does not rely on the perturbative diagram analysis. Combining it with the idea of variational cluster approach (VCA), we obtain an extended VCA theory. In this theory, both non-interacting and interacting part of the reference Hamiltonian can be varied to approach the stationary point of a generalized self-energy functional. In the limit of continuous bath degrees of freedom, it can recover the extended dynamical mean-field theory for non-local density-density interaction as well as the dynamical mean-field theory for correlated hopping. We also propose a VCA realization of the dynamical cluster approximation.

TT 16.84 Sa 11:00 Poster TU C

Dynamical local fields for quasiparticles — •Klaus Morawetz — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

The finite temperature dynamical response function including the dynamical local field is derived within a quasiparticle picture for interacting one-, two- and three dimensional Fermi systems. The correlations are assumed to be given by a density dependent effective mass, quasiparticle energy shift and relaxation time. The latter one describes disorder or collisional effects. This parameterization of correlations includes local density functionals as a special case and is therefore applicable for density functional theories. With a single static local field, the third order frequency sum rule can be fulfilled simultaneously with the compressibility sum rule by relating the effective mass and quasiparticle energy shift to the structure function or pair correlation function. Consequently, solely local density functionals without taking into account effective masses cannot fulfill both sum rules simultaneously with a static local field. The comparison to the Monte-Carlo data seems to support such quasiparticle picture.

[1] K. Morawetz, Phys. Rev. B 66 (2002) 07512

TT 16.85 Sa 11:00 Poster TU C

Time-Dependent Density Functional Theory of Disordered Metals — •V. G. Valeyev[1,2] and O. Pankratov[1] — [1]Lehrstuhl für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7/B2, 91058 Erlangen, Germany — [2]A. I. Alikhanov Institute for Theoretical and Experimental Physics, Bolshaya Cheremushkinskaya, 25, 117218 Moscow, Russia

Time-dependent density functional theory for the interacting electron system with disorder is developed using the Keldysh dynamical formulation, [1,2]. Allowing for the averaging of the partition function over the realizations of the disorder potential, this approach circumvents the averaging of the highly non-linear Kohn-Sham equation. Our main result is the novel formulation of TD DFT, where the electron and the current density, as well as the one-particle density of states are determined by the distribution function of the Kohn-Sham particles, naturally emerging from the Keldysh formalism. Introduction of the exchange-correlation potential in fact is an alternative method to solve the appropriate saddle-point equation, which has now a structure of the Vlasov-type kinetic equation for the Kohn-Sham distribution function with the exchange-correlation potential as a self-consistent field. The time-dependent OEP-approximation for the latter is derived, accounting for the diffusive motion of electrons in the system. It describes the low-temperature quantum interference phenomena in a disordered conductor with the long-ranged Coulomb interaction. References: [1] L.V. Keldysh, Zh. Eksp. Theor. Fiz. 47, 1515 (1964) [Sov. Phys. JETP 20, 1018 (1965)]. [2] A. Kamenev and A. Andreev, Phys. Rev. B60, 2218 (1999).

TT 16.86 Sa 11:00 Poster TU C

Full orbital LDA+DMFT scheme and its application to strongly correlated materials — •G. Keller[1], V. I. Anisimov[2], D. E. Kondakov[2], A. V. Kozhevnikov[2], I. A. Nekrasov[2], Z. V. Pchelkina[2], I. Leonov[1], X. Ren[1], and D. Vollhardt[1] — [1]Theoretische Physik III, Universität Augsburg, 86135 Augsburg — [2]Institut für Metallphysik, Ekaterinburg GSP-170, Russland

We discuss a recently developed full orbital LDA+DMFT scheme [1] in Wannier basis. The Hamiltonian $\hat{H}^{WF}$ for the partially filled bands of interest and the Coulomb interaction term between Wannier orbitals are obtained as *ab-initio* input to the correlation problem, which is then solved in DMFT(QMC). The interaction parameters for the DMFT(QMC) computations are calculated by constrained LDA. Subsequently, the self-energy matrix in Wannier basis, $\hat{\Sigma}(\varepsilon)$, can be converted back into full-orbital Hilbert space, and thus can be used to calculate the full-orbital interacting Green function $G(r, r', \varepsilon)$. The Green function can be also employed for the calculation of spectral, magnetic and electronic properties of the system. The results obtained with this method for $SrVO_3$ and V_2O_3 are compared with our previous results obtained with the LDA+DMFT with DOS input and with new bulk-sensitive experimental photoemission spectroscopy data [2,3,4].

[1] V.I. Anisimov *et al.*, cond-mat/0407359
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[3] S.-K. Mo *et al.*, Phys. Rev. Lett. **90**, 186403 (2003)
[4] G. Keller *et al.*, Phys. Rev. B **70**, 205116 (2004)

TT 16.87 Sa 11:00 Poster TU C

Self-consistent LDA+DMFT investigation of NiO — •X. Ren[1], I. Leonov[1], V. I. Anisimov[2], I. A. Nekrasov[2], G. Keller[1], and D. Vollhardt[1] — [1]Theoretische Physik III, Universität Augsburg, 86135 Augsburg — [2]Institut für Metallphysik, Ekaterinburg GSP-170, Russland

A recently proposed self-consistent LDA+DMFT scheme [1] is implemented. In this new scheme the feedback from DMFT to LDA which is absent in the conventional LDA+DMFT scheme, is made possible by employing the basis of Wannier functions (WFs) in the DMFT calculation. This improvement is desirable because the electron density on which the LDA band structure depends may be changed by the correlation effect introduced by DMFT. The electronic spectrum of NiO in the non-magnetic phase is calculated by both the new scheme and the conventional one, and a comparison is made.

TT 16.88 Sa 11:00 Poster TU C

A hydrostatic pressure cell for precise resistivity measurement above 7 GPa at low temperatures in magnetic fields — •Takeshi Nakanishi — Kompetenzgruppe Hohe Drücke, Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, D-01187 Dresden

We report recent developments in a new type of hydrostatic pressure cell [1] designed to measure the absolute value of the electrical resistivity in magnetic fields at low temperatures. This pressure cell, based on a technique using modified Bridgman anvils with a Teflon capsule that contains a liquid pressure transmitting medium, can generate nearly hydrostatic pressure at least up to $P \simeq 7.1$ GPa. The performance of this pressure cell was demonstrated by the electrical resistivity measurement on a single crystal of heavy fermion superconductor $CeCu_2(Si_{0.9}Ge_{0.1})_2$ at low temperatures down to $T = 50$ mK [2]. Pressure is controlled with high accuracy ($0 \leq P \leq 7$ GPa). Very recently, we have succeeded in generating a hydrostatic pressure of 7.7 GPa when a load of 74 kN ($\simeq 7.5$ ton) was applied. This implies a possibility that one can generate hydrostatic pressures above 10 GPa in the more compact size of this pressure cell. We present a modified design of the present pressure cell, which can be fitted to a commercial PPMS (Physical Property Measurement System, Quantum Design). [1] T. Nakanishi, N. Takeshita and N. Môri, Rev. Sci. Instrum. **73**, 1828 (2002). [2] T. Nakanishi, G. Sparn, H.S. Jeevan, M. Deppe, C. Geibel and F. Steglich, to be published in Proccedings of the International Conference on Strongly Correlated Electron Systems, Karlsruhe, Germany, July 26-30, 2004.

TT 16.89 Sa 11:00 Poster TU C

Resonant soft x-ray diffraction to study electronic order — •C. Schüssler-Langeheine[1], J. Schlappa[1], A. Tanaka[2], C.-F. Chang[1], Z. Hu[1], M. Benomar[1], H. Ott[1], E. Schierle[3], E. Weschke[3], G. Kaindl[3], M. Braden[1], and L. H. Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]ADSM, Hiroshima University, Japan — [3]Institut für Experimentalphysik, Freie Universität Berlin

Resonant diffraction in the soft x-ray range (RSXS) is a new tool, which is particularly suited to study superstructures formed by modulations of the electronic state, like differences in the valence or in the orbital occupation. Such kind of order can be found in various correlated-electron systems. RSXS as a combination of spectroscopy and diffraction is based on the strong sensitivity of resonances in the soft x-ray range, namely the transition-metal $2p \rightarrow 3d$, oxygen $1s \rightarrow 2p$ and lanthanide

$3d \rightarrow 4f$ excitations, on details of the electronic state. This sensitivity leads to different scattering cross sections for sites with different electronic configurations and creates a photon-energy dependent contrast for the diffraction process. Already on a qualitative level by comparison between the x-ray absorption spectrum and the energy dependence of the diffracted intensity, signatures of electronic order can be detected. Furthermore, since resonances in the soft x-ray range are well understood, a detailed microscopic modeling of the resonant diffraction is feasible, providing direct spectroscopic information about the ordered part of the system.

TT 16.90 Sa 11:00 Poster TU C

Status of the WERA Soft X-Ray Beamline at ANKA — •Eric Pellegrin, Peter Nagel, Bernd Scheerer, and Stefan Schuppler — Forschungszentrum Karlsruhe, IFP, Postfach 3640, 76021 Karlsruhe, Germany

After its commissioning in early 2005, the WERA beamline at the 2.5 GeV ANKA synchrotron radiation facility within the Forschungszentrum Karlsruhe is to be used for classical as well as for advanced electron spectroscopy in the photon energy range between 80 and 1400 eV (with a later extension down to about 15 eV photon energy). The main objective of WERA is to provide the user with most of the presently available electron spectroscopy tools in situ in order to allow a complete characterization of the electronic as well as the magnetic structure of the sample under investigation. Thus, versatility (instead of specialization) is the primary goal for WERA.

The following experimental stations will be available (incl. an in situ sample transfer between the individual experimental setups) together with the corresponding sample preparation chambers:

-photoemission electron microscopy

-photoemission spectroscopy, resonant photoemission spectroscopy, near-edge x-ray absorption spectroscopy

-soft x-ray magnetic circular dichroism (planned)

-pulsed laser deposition of epitaxial thin film samples

The technical specifications, the status and the future developments of the WERA soft x-ray beamline project will be presented.

TT 16.91 Sa 11:00 Poster TU C

Strukturdynamik und thermisches Rauschen von optischen Komponenten für Gravitationswellendetektoren — •Anja Zimmer, Ronny Nawrodt, Sandor Nietzsche, Ralf Neubert, Matthias Thuerk, Wolfgang Vodel und Paul Seidel — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena

Zur direkten Messung der von Einstein vorausgesagten Gravitationswellen mittels interferometrischer Gravitationswellendetektoren ist es erforderlich, das thermische Rauschen optischer Komponenten wie Endspiegel und Strahlteiler zu senken. Wurden die Interferometer bisher bei Raumtemperatur betrieben, so könnte die Anwendung von Kryotechniken entscheidende Fortschritte bringen und somit die "Gravitationswellenastronomie" ermöglichen.

Die Arbeiten im Teilprojekt des gleichnamigen von der DFG geförderten Sonderforschungsbereiches TR7 zielen insbesondere auf die experimentelle Untersuchung der in den optischen Komponenten zu Dämpfungsverlusten (und damit zu thermischem Rauschen) führenden Prozesse. Eine entscheidende Rolle dabei spielt die numerische Simulation der Strukturdynamik der optischen Komponenten, mit deren Hilfe sich das Schwingungsverhalten der Testkörper hinsichtlich Substratmaterial, Beschichtung und Strukturierung optimieren lässt. Neben den aktuellen Ergebnissen dieser FEM-basierten Simulationen werden wesentliche kryotechnische Aspekte eines speziellen Messaufbaus zur experimentellen Bestimmung der mechanischen Güte von optischen Komponenten im Temperaturbereich von 300 K bis zu 5 K diskutiert.

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Neuartige Blei-Regeneratormaterialien für Kleinkältemaschinen im Temperaturbereich unterhalb 60 K — •Torsten Koettig, Stefan Moldenhauer, Matthias Thuerk und Paul Seidel — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena

Traditionelle Regeneratormaterialien wie Edelstahl- und Bronzedrahtsiebgewebe erreichen in ein- und zweistufigen Kleinkältemaschinen unterhalb von 30 K ihre Leistungsgrenze. Wegen seiner höheren Wärmekapazität wird in diesem Temperaturbereich Blei eingesetzt. Die bisher übliche Kugelform des Regeneratormaterials begrenzt Regeneratorkenngrößen wie Porosität und Druckverlust auf thermodynamisch nicht optimale Bereiche. Die notwendige Fixierung des Bleipulvers im Festbett erfordert zusätzlichen technologischen Aufwand. Es ist gelungen ein Bleisiebgewebe mit variablen Dimensionen herzustellen. Dadurch können auch Bleiregeneratoren hinsichtlich Ihrer inneren Parameter wie mesh-Zahl, Drahtdurchmesser oder Oberflächenrauhigkeit thermodynamisch optimiert werden. Die Möglichkeiten zur Verbesserung der Regeneratoreigenschaften des Bleidrahtgewebes gegenüber traditionellen Bleipulverregeneratoren werden diskutiert. Das Leistungspotenzial des Materials wird am Beispiel eines einstufigen Pulsationsröhrenkühlers demonstriert. Insbesondere erreicht dieser stark verbesserte Kälteleistungen unterhalb von 30 K ohne die üblichen Leistungsverminderungen bei höheren Kühltemperaturen über 60 K aufzuweisen.