TT 20: Correlated Electrons - Poster Session

Time: Wednesday 14:00–17:45 Location: Poster A

TT 20.1 Wed 14:00 Poster A

Neutron Scattering and X-ray Diffraction on $HoInCu_4$ — •Veronika Fritsch[1,3], Svilen Bobev[2], John L. Sarrao[3], Uwe Amann[4,5], and Oliver Stockert[6] — [1]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Department of Chemistry, University of Delaware, Newark, DE 19716, USA — [3]Los Alamos National Laboratory, Los Alamos, NM 87545, USA — [4]BENSC, HMI, 14109 Berlin, Germany — [5]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [6]MPI-CPfS, 01187 Dresden, Germany

The ternary rare-earth compounds $R\mathrm{InCu}_4$ (R = Gd, Dy, Ho and Er) show strong indications of frustration as manifested by measurements of magnetic susceptibility and specific heat. The crystal structure, in which the rare-earth ions occupy a face-centered cubic lattice, suggests the presence of geometrical frustration. In order to get further insight into the crystal and magnetic structure we performed X-ray diffraction measurements on flux-grown single crystals and neutron diffraction measurements on powder of $HoInCu_4$. Single crystal X-ray diffraction data confirmed that the samples are fully ordered, all atoms occupy crystallographically independent sites and crystallize in the cubic $AuBe_5$-structure. $HoInCu_4$ exhibits magnetic order below $T_N = 0.75$ K as evidenced by heat capacity measurements. Neutron diffraction patterns were taken above and below the Néel temperature, indicating a commensurate magnetic structure with a propagation vector $\tau = (1\ 1/2\ 0)$ below T_N as well as strong magnetic correlations in the paramagnetic state as expected in systems with strong frustration.

TT 20.2 Wed 14:00 Poster A

Spin Dynamics of $EuCu_2(Ge_{(1-x)}Si_x)_2$ probed by Electron Spin Resonance — •Tobias Foerster[1], Joerg Sichelschmidt[1], Zakir Hossain[2], and Christoph Geibel[1] — [1]Max Planck Institut f. Chemische Physik Fester Körper, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Department of Physics, Indian Institut of Technology, Kanpur, India

The intermetallic alloy $EuCu_2(Ge_{(1-x)}Si_x)_2$ can be used to investigate the transition from divalent antiferromagnetic state to the valence fluctuating state of Eu. By tuning x one observes an antiferromagnetic ordered state which is stable up to $x_c \approx 0.65$. For $x > 0.5$ the system shows valence fluctuation behaviour. Additionally, for $x > 0.4$ Kondo-like behaviour appears, becoming pronounced around x_c where also heavy Fermi liquid formation is observed.
We investigated polycrystalline samples of $EuCu_2(Ge_{(1-x)}Si_x)_2$ ($0 \leq x \leq 1$) by Electron Spin Resonance (ESR) at X-Band frequencies. All compositions show well defined ESR spectra at a g-factor typical for Eu^{2+} ions. We observe different temperature dependencies of the line width in different regions of the phase diagram. For example the sample with $x = 0.6375$ shows a line width increase for rising temperature with a change of slope near the estimated Kondo temperature, $T_K \approx 30K$. This behaviour is very similar to the pattern observed for ESR probe spins embedded in a Kondo lattice system. The ESR spectra are analyzed concerning the backround of bulk measurements.

TT 20.3 Wed 14:00 Poster A

Boron induced change of valence state of Eu in $EuPd_3B_x$ ($0 \leq x \leq 0.55$) — •Roman Gumeniuk, Claire Loison, Andreas Leithe-Jasper, Walter Schnelle, Ulrich Burkhardt, Marcus Schmidt, Miriam Schmitt, Ulrich Schwarz, and Helge Rosner — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

A detailed experimental and theoretical study of the solubility of B in cubic $EuPd_3$ ($AuCu_3$ structure type) and its influence on the physical properties is presented here. Theoretical calculations (LDA + U + CPA method) predict in $EuPd_3B_x$ a change of non-magnetic $4f^6$ Eu to magnetic $4f^7$ Eu for a boron content of $x > 0.2$ together with an anomaly in the unit cell volume. At 950°C the incorporation of B in the structure of $EuPd_3B_x$ is possible up to $x = 0.55$, as can be concluded from measurements of lattice parameters, WDXS and chemical analyses. The lattice parameter of $EuPd_3B_x$ varies linearly with B content (x) with a distinct change of slope at $x = 0.31$. From Eu L_{III} XAS studies as well as from measurements of magnetic susceptibility it can be deduced that Eu atoms in $EuPd_3$ and in $EuPd_3B_x$ ($0 \leq x \leq 0.31$) exhibit a $4f^6$ state, while for $EuPd_3B_x$ ($0.31 \leq x \leq 0.55$) an intermediate valence state of (mixed $4f^6$ and $4f^7$) can be assumed. Our findings are discussed with respect to previously published studies [1,2].
[1] B. Darshan *et al.* Phys. Rev. B **30** (1984) 4031-4033.
[2] S. K. Dhar *et al.* Phys. Rev. B **29** (1984) 5953-5956.

TT 20.4 Wed 14:00 Poster A

Coexistence of ferromagnetism and underscreened Kondo effect in uranium compounds — •Natalia Perkins[1], Jose Roberto Iglesias[2], and Bernard Coqblin[3] — [1]Technische University of Braunschweig, Braunschweig,38106, Germany — [2]Instituto di Fisica, Universidade Federal do Rio Grand do Sul, 91501-970, Porto Alegre, Brazil — [3]Laboratoire de Physique des Solides, Universite Paris-Sud, Batiment 510, 91405 Orsay, France

Coexistence between ferromagnetic order and Kondo behavior has been experimentally observed in some uranium compounds, like UTe or UCu0.9Sb2. This is an unusual behavior as Kondo effect generally compete with magnetic order, for instance in Ce compounds. Here we propose underscreened Kondo lattice model, including localized S=1 spins which couple to conduction electron through an on-site Kondo coupling, while interacting among them ferromagnetically. Results are obtained for different temperatures and values of the band filling and they show that the Kondo temperature is larger than the Curie temperature, suggesting a scenario for the coexistence of Kondo effect and ferromagnetic order.

TT 20.5 Wed 14:00 Poster A

Detailed studies of the resistive superconducting transition in UNi_2Al_3 thin films — •Michael Foerster, Martin Jourdan, Andrey Zakharov, and Hermann Adrian — Johannes Gutenberg-Universität, Institut für Physik, Mainz, Germany

Some time ago a dependence of the resistive superconducting transition temperature on the current direction in UNi_2Al_3 thin films was observed. Although a qualitative explanation can be given, fundamental questions about this phenomenon are still open, which motivated more detailed studies.

Morphological investigations by AFM and STM seem to rule out a growth mechanism induced origin. By using a specially designed photomask we were able to measure the transition down to current densities of 0.1 A/cm^2 and observed no vanishing of the difference in T_c. However, the magnitude of the splitting of the sc transition varies from sample to sample without any correlation to the defect density as determined by the residual resistance ratio. V(I) characteristics in the superconducting state were measured at various magnetic fields, indicating anisotropic pinning. For the current direction I‖c a thermally activated flux flow region could be identified.

Additional measurements with higher current densities prove that the observations in the relevant range are not generated by heating effects. The shift in T_c as a function of current density agrees well with the expectation for pairbreaking critical current from Ginzburg-Landau theory.

TT 20.6 Wed 14:00 Poster A

Magnetic order in $CeIn_{3-x}Sn_x$ investigated by μSR measurements — •Julia Arndt[1], Astrid Schneidewind[2], Oliver Stockert[1], Daniel Andreica[3], Nubia Caroca-Canales[1], Christoph Geibel[1], and Michael Loewenhaupt[2] — [1]MPI f. Chemische Physik fester Stoffe, D-01187 Dresden — [2]Inst. f. Festkörperphysik, TU Dresden, D-01062 Dresden — [3]Laboratory for Muon Spin Spectroscopy, PSI, CH-5232 Villigen

We report on zero-field muon spin rotation (μSR) measurements on single crystals of the cubic heavy-fermion compound $CeIn_{3-x}Sn_x$. $CeIn_3$ orders antiferromagnetically below $T_N = 10.2$ K. Substituting Sn for In suppresses the magnetic order until $T_N = 0$ at a critical concentration $x_c = 0.67$ [1]. For $x < 0.2$ the specific heat C exhibits the typical λ shaped anomaly at T_N, whereas for $x > 0.2$ C shows a broad maximum in the vicinity of the phase transition, which is taken as a sign for a change in the magnetic structure [2]. So far it has not been accomplished to detect magnetic intensity by means of neutron scattering in this region [3]. In contrast, μSR with its sensitivity to small local magnetic fields in the sample gives the opportunity to probe if magnetic order is present for $x > 0$ at all. All $CeIn_{3-x}Sn_x$ samples investigated ($x = 0; 0.2; 0.4; 0.55$) show a Kubo-Toyabe shaped μSR signal with

high depolarisation below T_N and very weak damping above. This is interpreted as the first detection of a clear signature of magnetic order in $CeIn_{3-x}Sn_x$ for $x > 0$.
[1] T. Rus *et al.*, Physica B, **359-361**, 62 (2005); [2] P. Pedrazzini *et al.*, Eur. Phys. J. B, **38**, 445 (2004); [3] O.Stockert *et al.*, unpublished

TT 20.7 Wed 14:00 Poster A

Deposition of $CeCoIn_5$ thin films by co-sputtering and evaporation — •Jochen Geerk[1], Alexander Zaitsev[1], Rainer Fromknecht[1], Andre Beck[1], and Hilbert v. Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.B. 3640, D-76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe

Thin films of the heavy fermion superconductor $CeCoIn_5$ were prepared on sapphire substrates with different orientations by combining sputtering (Ce and Co) and evaporation (In). The sputter targets of Ce and Co were arranged in a face-to-face geometry with a magnetic field applied perpendicular to the target surface thus providing an oscillatory movement of the secondary electrons between the targets the latter acting as electric mirrors. Indium was evaporated from a BN oven. In the course of our studies the composition of the films, controlled by RBS and EDX, was varied between ± 30 % for the three elements and the growth temperature ranged from 500 to 750 ° C. The films obtained so far showed transition temperatures between 1.5 and 2.0 K and the characteristic maximum in resistivity near 40 K.

TT 20.8 Wed 14:00 Poster A

High pressure resistivity studies on $YbIr_2Si_2$ — •Monica Macovei[1], Michael Nicklas[1], Cornelius Krellner[1], Zakir Hossain[2], Christoph Geibel[1], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01069 Dresden, Germany — [2]Departament of Physics, Indian Institute of Technology, Kampur 208016, India

We investigated the high pressure phase diagram on high-quality single crystals of $YbIr_2Si_2$. Electrical resistivity,ρ, was measured in the pressure range up to 10 GPa and for temperature 0.05 K $< T <$ 300 K. Ambient pressure specific heat and resistivity studies confirmed a Fermi liquid ground state below $\sim$ 200 mK [1]. The Fermi liquid ground state is persisting at low pressure $p < 2$ GPa. However, with further increasing pressure the low-temperature dependence of the resisitivity changes from a T^2 dependence to $\rho = \rho_0 + AT^n$ with $n < 2$, indicating non-Fermi liquid behavior. By applying a magnetic field the Fermi liquid ground state is stabilized again. For $p > 7$ GPa magnetic order is developing marked by a kink in resistivity similar like in other Yb based heavy fermion compounds, e.g. $YbRh_2Si_2$, $YbCu_2Si_2$ and $YbNi_2Ge_2$.
[1] Z.Hossain *et al.* Phys. Rev. B **72**, 094411 (2005).

TT 20.9 Wed 14:00 Poster A

$YbNi_2Si_3$: a new Yb based intermetallic compound — Alexander Cosceev[1], Marc Uhlarz[1], Thomas Wolf[2], Peter Adelmann[2], •Kai Grube[2], Peter Schweiss[2], Georg Roth[3], Rainer Fromknecht[2], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Physikalisches Institut, Universität Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, Germany — [3]Institut für Kristallographie, RWTH Aachen, Germany

We have synthesized a new intermetallic compound $YbNi_2Si_3$ which crystallizes in the space group $Immm$ with the metric $a = 3.860$Å, $b = 3.862$Å, and $c = 24.068$Å. Single crystals have been grown from Sn flux in a closed SiO_2 glass ampoule. Clean free-standing crystals could be obtained after dissolving the solid flux with liquid gallium and cleaning with a solution of iodine in dimethyl formamide. The magnetic dc susceptibility was measured parallel and perpendicular to the c axis. We find a rather strong anisotropy of the Curie-Weiss-like susceptibility down to 2.3 K. Measurements of the specific heat will be reported as well.

TT 20.10 Wed 14:00 Poster A

High-field ESR on the Kondo-system $YbRh_2Si_2$ — •Uwe Schaufuss[1], V. Kataev[1], B. Büchner[1], J. Sichelschmidt[2], C. Krellner[2], C. Geibel[2], and F. Steglich[2] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden — [2]Max Planck Institute for Chemical Physics of Solids, Dresden

$YbRh_2Si_2$ is a Kondo–system with a Kondo temperature $T_K \sim 25$ K [1] . It is located very close to a quantum critical point related to a very weak AFM order below $T_N = 65$ mK and a critical magnetic field of $B_C = 0.06$ T at ambient pressure. Surprisingly an ESR signal typical of a local Yb^{3+} spin has been observed below T_K at fields $B \leq 0.7$ T [2] . The occurrence of the ESR signal is unexpected because at $T \ll T_K$ the Yb^{3+} moments should be screened. In order to obtain a deeper insight in this unusual behaviour we have performed ESR measurements on single crystals of $YbRh_2Si_2$ at much higher fields (5 to 7.5 T) at temperatures from 3 to 25 K, i.e. in the region where one expects a crossover from a Non–Fermi liquid(NFL) to a Fermi–liquid (FL) phase [3] . We observe a strongly anisotropic signal which can be assigned to Yb^{3+} moments. The signal exhibits a pronounced dependence on temperature and the magnetic field. We discuss the puzzling controversy between the observation of ESR which shows properties characteristic of a local Yb^{3+} moment and the Kondo state of $YbRh_2Si_2$.
1 O. Trovarelli *et al.*: Phys. Rev. Lett. **85,** 626 (2000)
2 J. Sichelschmidt *et al.*: Phys. Rev. Lett. **91,** 156 401 (2003)
3 K. Ishida *et al.*: Phys. Rev. Lett. **89,** 107 202 (2002)

TT 20.11 Wed 14:00 Poster A

Magnetotransport across the field-induced quantum phase transition in $CeCu_{5.8}Au_{0.2}$ — •Marc Uhlarz[1], Moritz Röger[1], Tihomir Tomanic[1], and Hilbert v. Löhneysen[1,2] — [1]Physikalisches Institut, Universität Karlsruhe (TH), D-76128 Karlsruhe — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

We report on magnetoresistivity and Hall effect of $CeCu_{0.58}Au_{0.2}$, magnetic field B applied along the hard direction (b axis in orthorhombic notation) and current I along the a axis. At $B = 0$, $CeCu_{0.58}Au_{0.2}$ orders antiferromagnetically below $T_N = 0.25$ K [1]. As observed previously [1], the longitudinal electrical resistivity $\rho_{xx}(T)$ rises towards lower T below T_N for current directions containing a component of the magnetic ordering vector $\mathbf{Q} = (0.625, 0, 0.275)$. With increasing B, the rise of $\rho_{xx}(T)$ becomes smaller and T_N shifts to lower T, vanishing at $B_c = 3.6$ T. Likewise, the field derivative of the transverse resistivity $\mathrm{d}\rho_{xy}/\mathrm{d}B$ (independent of B at high temperatures) becomes field-dependent in the vicinity of B_c below T_N. This signals (in a simple single-band picture) an increase of the effective carrier concentration when B exceeds the critical field B_c of antiferromagnetic order. Our data will be compared to recent experiments on $YbRh_2Si_2$, where a kink of the Hall coefficient R_H at B_c was inferred for $T \to 0$ from the gradual change of slope of $\rho_{xy}(B)$ for finite T, becoming more pronounced for $T \to 0$ [2].
[1] H. v. Löhneysen et al., Eur. Phys. J. B **5** (1998) 447
[2] S. Paschen et al., Nature **432** (2004) 881.

TT 20.12 Wed 14:00 Poster A

DC-Susceptibility of $CeCu_{6-x}Au_x$ at very low temperatures — •Andreas Hamann[1], Tihomir Tomanic[1], Hilbert v. Löhneysen[1,2], and Oliver Stockert[3] — [1]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe — [3]MPI für chemische Physik fester Stoffe, 01187 Dresden

$CeCu_6$ is a prototype heavy-fermion system that is rather well described by Fermi liquid (FL) theory. Au doping introduces long-range incommensurate antiferromagnetism for $x > x_c \approx 0.1$. In the vicinity of the quantum critical point x_c significant deviations from FL theory have been observed in measurements of the specific heat, magnetic susceptibility and the electrical resistivity. In addition, highly unusual features were observed in inelastic neutron scattering [1,2]. In particular, the energy integrated dynamical as well as the statical susceptibility could be described by $\chi^{-1} \propto (\theta(q))^\alpha + cT^\alpha$ with $\alpha = 0.75$ [1]. We report measurements of the low-field dc-susceptibility $\chi(T)$ of $CeCu_{5.9}Au_{0.1}$ and $CeCu_{5.85}Au_{0.15}$ down to temperatures around 40 mK. Our data for $x = 0.1$ show for $T \lesssim 200$ mK deviations from the above χ^{-1} expression signaling a crossover for a smaller exponent α than previously found for higher T and B. For $x = 0.15$ we see clear experimental evidence for the sharp onset of antiferromagnetic order below $T_N \approx 82$ mK for $x = 0.15$. We compare our data in detail with the previous work [1].
[1] A. Schröder et al., Nature 407, 6802 (2000)
[2] O. Stockert et al., Phys. Rev. Lett. 80, 5627 (1998)

TT 20.13 Wed 14:00 Poster A

Quantenphasenübergänge in $NbFe_2$ — •Carsten Albrecht[1], Manuel Brando[2], Will Duncan[1], Dennis Moroni-Klementowicz[1], Daniel Grüner[2], Rafik Ballou[3], Bjorn Fak[4],

Guido Kreiner[2] und F. Malte Grosche[1] — [1]Dept. of Physics, Royal Holloway, University of London, Egham, UK — [2]MPI-CPfS, Nöthnitzer Str. 40, Dresden — [3]CNRS, Grenoble — [4]CEA DRFMC, SPSMS, Grenoble

Was geschieht mit metallischen Ferromagneten bei Annäherung an ihren quantenkritischen Punkt (QKP), wenn der magnetische Übergang kontinuierlich unterdrückt wird?

In einigen bisher untersuchten Fällen, insbesondere den stoichiometrischen Verbindungen MnSi und $ZrZn_2$, verdeckt die Wandlung zu Phasenübergängen 1. Ordnung den erwarteten QKP. Ein anderes Szenario wird möglicherweise in dem verwandten System $NbFe_2$ realisiert: $NbFe_2$ existiert dicht an der Schwelle zum Ferromagnetismus, erkennbar an seinem stark erhöhten Stonerfaktor $\simeq 120$ (bezogen auf die gerechnete Zustandsdichte), nimmt aber unterhalb von etwa 20 K vermutlich eine bisher nicht genau identifizierte Spindichtewellenordnung an. Sowohl leichter Fe- als auch leichter Nb- Überschuss im Bereich von einem Prozent führen zu itinerantem Ferromagnetismus. Unsere Untersuchungen an Proben aus den bisher identifizierten Bereichen des Zusammensetzungs-Phasendiagramms sowie eine Reihe von Hochdruckmessungen weisen darauf hin, dass in $NbFe_2$ der ferromagnetische QKP durch Wandlung von Ferromagnetismus zu langwellig modulierter Spindichtewellen- bzw. Spiralordnung verdeckt wird.

TT 20.14 Wed 14:00 Poster A

Magnetic-field-induced Change of the Fermi Surface in CeBiPt — •M Bartkowiak[1], B Bergk[1], Y Skourski[1], J Wosnitza[1], I Opahle[2], S Elgazzar[2], M Richter[2], H v Löhneysen[3,4], T Yoshino[5], and T Takabatake[5] — [1]Hochfeld-Magnetlabor Dresden (HLD) FZ Dresden-Rossendorf, 01328 Dresden — [2]IFW Dresden,PO Box 270116, 01171 Dresden — [3]Physikalisches Institut, Universität Karlsruhe — [4]Institut für Festkörperphysik, FZ Karlsruhe — [5]Department of Quantum Matter, ADSM, Hiroshima University

Comparative experiments between the two semimetals CeBiPt and LaBiPt reveal changes of the Fermi surface in CeBiPt with respect to temperature, applied magnetic, field and chemical composition. It must be concluded that the strong temperature dependence of the Shubnikov-de Haas (SdH) frequency as well as the change of carrier concentration above a sample dependent critical field are associated with the $4f$ electrons introduced by the Ce atoms. We present Hall and magnetoresistance measurements up to 70 T obtained at our new pulsed high magnetic field laboratory in Dresden. We observe the disappearance of the SdH signal and a change of the Hall coefficient above a sample-dependent threshold field. Rather than at 25 T, as reported previously, we measured a threshold field of ≈ 40 T demonstrating the strong dependence of the Fermi surface on stoichiometry.

TT 20.15 Wed 14:00 Poster A

Inelastic Neutron Scattering on the Antiferromagnetic Half-Heusler Alloy CeBiPt — •Gernot Goll[1], Oliver Stockert[2], Tobias Unruh[3], Peter Link[3], K. Shigetoh[4], and T. Takabatake[4] — [1]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe — [2]Max-Planck-Institut CPfS, 01187 Dresden — [3]ZWE FRM-II, Technische Universität München, 85747 Garching — [4]Hiroshima University, Higashi-Hiroshima, Japan

CeBiPt is a semimetal with a rather low charge carrier concentration $n = 7.7 \cdot 10^{17}\,\mathrm{cm}^{-3}$. Below $T_\mathrm{N} \approx 1$ K antiferromagnetic order occurres as evidenced by sharp maxima in the thermodynamic properties. Neutron diffraction experiments have revealed an AF-type I structure with a propagation vector $\tau = (1\ 0\ 0)$ and moments also along [1 0 0]. The ordered moment $\mu \approx 0.6\,\mu_\mathrm{B}$ is much lower than the effective moment determined from the Curie-Weiss behavior of the susceptibility at higher T. Crystal-electric field (CEF) splitting of the Ce^{3+} level might be one origin of a lowered ordered moment. We performed inelastic neutron scattering experiments on TOFTOF at the FRM-II with energy of the incident neutrons $E_i = 2.7$, 5.7, and 16.9 meV and on PANDA with $E_i = 5.6$ meV at $2.8 < T < 50$ K. We found only one CEF excitation at $\hbar\omega \approx 9.5$ meV at $T = 2$ K in line with previous measurements on SV29 at FRJ-2 with fixed $E_i = 30$ meV. This excitation has been identified with the transition between a Γ_7 doublet and a Γ_8 quartet state. No further inelastic excitations have been observed except for a quasielastic contribution which increases in width with increasing temperature.

TT 20.16 Wed 14:00 Poster A

Kondo effect in low-carrier systems — •Robert Hager and Ralf Bulla — Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg

Recent experiments on dilute U impurities in semiconducting CaB_6 show typical Kondo phenomena with a Kondo temperature $T_\mathrm{K} \approx 2K$ (G.A. Wigger *et al.*, Europhys. Lett. **68**, 685 (2004)). This observation is rather unusual for magnetic moments due to 5f electrons because of the large hybridization between impurities and the conduction electrons. We perform numerical renormalization group calculations for an Anderson impurity model with a low concentration of conduction electrons, believed to be the relevant model for $(U,Ca)B_6$. We present results for thermodynamic and dynamic quantities for various carrier concentrations and investigate the crossover from mixed-valent to Kondo behaviour upon decreasing the filling of the conduction band.

TT 20.17 Wed 14:00 Poster A

Strong inhomogeneities and non-Fermi liquids in randomly depleted Kondo lattices — •Matthias Vojta[1] and Ribhu Kaul[2] — [1]Institut für Theoretische Physik, Universität Köln — [2]Physics Department, Harvard University

We discuss the low-temperature behavior of Kondo lattices upon random depletion of the local f moments. For a large range of intermediate doping levels, between the coherent Fermi liquid of the dense lattice and the single-impurity Fermi liquid of the dilute limit, we find strongly inhomogeneous states that exhibit distinct non-Fermi liquid characteristics. In particular, the interplay of dopant disorder and strong interactions leads to rare weakly screened moments which dominate the bulk susceptibility. Our results are relevant to compounds like $(Ce,La)CoIn_5$.

TT 20.18 Wed 14:00 Poster A

Unusual Single Ion Behavior in $CeNi_{8.6}Cu_{0.4}Ge_4$ near a Quantum Critical Phase Transition — •Ludwig Peyker[1], Ernst-Wilhelm Scheidt[1], Wolfgang Scherer[1], Stephan Kehrein[2], and Herwig Michor[3] — [1]Chemische Physik und Materialwissenschaften, Universität Augsburg, 86159 Augsburg, Germany — [2]Fakultät für Physik, LMU München, 80333 München, Germany — [3]Institut für Festkörperphysik, TU Wien, 1040 Wien, Austria

We report on specific heat and magnetic susceptibility measurements of the heavy fermion intermetallic system $CeNi_{9-x}Cu_xGe_4$ for various concentrations ranging from the stoichiometric compound with $x = 0$ to $x = 1$. $CeNi_9Ge_4$ reveals the largest ever recorded value of the electronic specific heat $\Delta C/T \approx 5.5\,\mathrm{J\,K^{-2}mol^{-1}}$ at $T = 80$ mK without any magnetic order. This behavior is mainly driven by single ion (Ce) effects due to the competition between Kondo effect and crystal electrical field splitting [1]. Changing the environment of the magnetic ion Ce by replacing Ni with Cu leads to a long range antiferromagnetic order at $T_\mathrm{N} = 180$ mK for $CeNi_8CuGe_4$. In between $CeNi_{8.6}Cu_{0.4}Ge_4$ reveals a logarithmic temperature dependency in specific heat indicating non Fermi liquid behavior. This behavior will be discussed in a quantum critical phase transition scenario.

[1] U. Killer, E.-W. Scheidt, G. Eickerling, H. Michor, J. Sereni, Th. Pruschke, S. Kehrein, Phys. Rev. Lett. **92**, 27003 (2004)

TT 20.19 Wed 14:00 Poster A

Matrix Product States for comparing NRG to DMRG — •Hamed Saberi, Andreas Weichselbaum, and Jan von Delft — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Munich, Germany

Wilson's Numerical Renormalization Group (NRG) method for solving quantum impurity models can be turned into a variational method within the set of so-called Matrix Product States (MPS) with much more flexibility and efficient use of numerical resources. Since White's Density Matrix Renormalization Group (DMRG) for treating quantum lattice problems can likewise be reformulated in terms of MPSs, the NRG and DMRG are now seen to have the same formal basis, namely both are built on MPS. This enables us to compare the NRG approach for the Single Impurity Anderson model to the DMRG approach and also to see how NRG results can be improved upon systematically by performing a variational optimization in a space of variational matrix product states of the same structure as those used by NRG.

TT 20.20 Wed 14:00 Poster A

Coupled-Cluster Method for the Anderson Impurity Model — •Jin-Jun Liang, Clive Emary, and Tobias Brandes — Sekr. PN 7-1, Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 BERLIN-Charlottenburg

The coupled-cluster method (CCM) is one of the most powerful and numerically accurate approximation method for describing many-body

systems. It is popular in nuclear physics, quantum chemistry and quantum magnetism. However, the method has been rarely applied to the Anderson impurity model. Here with CCM, we calculate the model's energies and wave-functions for the ground state as well as some excited states. Results are compared with those from other methods, including self-consistent perturbation and variational methods.

TT 20.21 Wed 14:00 Poster A

Quantum Monte-Carlo scheme for the solution of the Kondo impurity problem with an arbitrary density of free electron states — •Evgeny Gorelov[1,2], Andrey Zhuravlev[1,3], Alexey Rubtsov[4], and Alexander Lichtenstein[1] — [1]I. Institut für theoretische Physik, Universität Hamburg, Jungiusstrasse 9, 20355 Hamburg — [2]Theoretical Physics and Applied Mathematics Department, Urals State Technical University, Mira Street 19, 620002 Ekaterinburg, Russia — [3]Institute of Metal Physics, 620219 Ekaterinburg, Russia — [4]Department of Physics, Moscow State University, 119992 Moscow, Russia

The numerically exact determinantal continuous time QMC method has been applied to calculate properties of a Kondo impurity coupled to a band of free electrons with an arbitrary density of states (DOS). This approach allows to calculate spin susceptibilities as well as Green functions, accurately taking into account all the peculiarities of the free electron DOS. The method was applied to a Kondo impurity embedded into different environments: ultrasmall grain, Anderson model (lattice with random on-site energy levels) and a 2-dimensional lattice, where the DOS has a van Hove singularity.

TT 20.22 Wed 14:00 Poster A

Correlation Functions in the Non-Equilibrium Anisotropic Kondo Model — •Peter Fritsch and Stefan Kehrein — Physics Department, ASC, and CeNS, Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 Munich, Germany

In this work we investigate the spin-spin correlation function in the Anisotropic Kondo Model using the method of infinitesimal unitary transformations (flow equations) [1]. We derive a perturbative scaling picture of the model which allows us to study the long-time evolution of observables. Within this framework we are able to study the effect of both equilibrium and non-equilibrium (dc voltage bias) decoherence on the physical properties of this model.

Future plans include the investigation of the Kondo Model in a magnetic field. This work is a generalization of the previous flow equation analysis of the non-equilibrium Kondo Model [2] for systems without SU(2)-symmetry.

[1] S. Kehrein, The Flow Equation Approach to Many-Particle Systems, Springer Tracts in Modern Physics 217

[2] S. Kehrein, Phys. Rev. Lett. 95, 056602 (2005)

TT 20.23 Wed 14:00 Poster A

High-Field NMR Relaxation Rates in Spin-1/2 Heisenberg-Chains — •Simon Grossjohann[1], Wolfram Brenig[1], Hannes Kühne[2], and Hans-Henning Klauss[2] — [1]Institut für Theoretische Physik, Technische Universität Braunschweig, D-31806 Braunschweig, Germany — [2]Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, D-38106 Braunschweig, Germany

We study the critical dynamics of the one-dimensional antiferromagnetic spin-1/2 Heisenberg chain across the field-driven quantum phase transition into the fully polarized state at saturation field. Using a Quantum-Monte-Carlo approach based on the the Stochastic Series Expansion we evaluate the low-temperature transverse and longitudinal imaginary-time spin-correlation functions and perform analytic continuation to the frequency domain by Maximum-Entropy methods. Results will be presented in the thermodynamic limit for the temperature T, magnetic-field B, and momentum dependence of the dynamic structure factor. In particular we analyze these results in terms of the transverse nuclear-magnetic relaxation time $T_1(T, B)$. We observe a clear signature of quantum critical slowing-down, leading to an enhanced relaxation in the vicinity of the saturation field as well as relaxation from gapful excitations only above criticality. Finally, we compare our calculations with recent high-field $1/T_1$ NMR-data as observed on CuPzN and find satisfying agreement for all temperatures and magnetic fields investigated.

TT 20.24 Wed 14:00 Poster A

Quantum Critical Spin Dynamics of a Cu(II) S=1/2 antiferromagnetic Heisenberg chain studied by ^{13}C-NMR spectroscopy — •H. Kühne[1], J. Litterst[1], H.-H. Klauss[1], S. Grossjohann[2], W. Brenig[2], A.P. Reyes[3], P.L. Kuhns[3], C.P. Landee[4], M.M. Turnbull[4], H.-J. Grafe[5], J. Haase[5], and B. Büchner[5] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig — [2]Institut für Theoretische Physik, TU Braunschweig — [3]NHMFL, FSU, Tallahassee, USA — [4]DPC, Clark University, Worcester, USA — [5]Leibnitz-Institut für Werkstoffforschung, Dresden

The antiferromagnetic S=1/2 Heisenberg chain is a model system for quantum many-body physics. It allows a direct comparison between exact theoretical results and experiment for ground state properties and excitations. $Cu(C_4H_4N_2)(NO_3)_2$ (CuPzN) is a very good experimental realization of an unperturbed S=1/2 chain [1,2]. In this compound we study the low energy spin dynamics of a Cu(II) S=1/2 spin chain system by means of NMR. We measured the nuclear spin-lattice relaxation rate of ^{13}C as a function of temperature in a wide external magnetic field range from 2T-22T, with an emphasis on the critical field range around 15T. The experimental data are in very good agreement with Quantum Monte Carlo calculations and clearly show the crossover from quantum critical behavior at low temperatures to diffusive modes at elevated temperatures.[1] P. Hammar et al., PRB. 59, 1008 (1999). [2] M.B. Stone et al., PRL 91, 037205 (2003).

TT 20.25 Wed 14:00 Poster A

Magnetic properties and evidence for lattice instabilities of the frustrated 2D s=1/2 systems (CuCl)$LaNb_2O_7$ and (CuBr)$LaNb_2O_7$. — •Patric Scheib[1], Vladimir Gnezdilov[2], Peter Lemmens[1], Yuri Georgii Pashkevich[3], Kazuyoshi Yoshimura[4], Yoshitami Ajiro[4], Taro Kitano[4], and Hiroshi Kageyama[4] — [1]Institut für Physik der kondensierten Materie, TU-Braunschweig, Braunschweig — [2]Institute for Low Temperature Physics and Engineering, NASU, Kharkov, Ukraine — [3]Donetsk Phystech, NASU, Ukraine — [4]Department of Chemistry, Kyoto University, Kyoto, Japan

We report on the magnetic properties and raman scattering data of the double-layered perovskites (CuBr)$LaNb_2O_7$ and (CuCl)$LaNb_2O_7$ with a square lattice of $s = \frac{1}{2}$ prepared by topotactic ion-exchange reactions. Evidence for competing ferro- and antiferromagnetic exchange pathes connecting nearest and second-nearest-neighbors, respectively, exist. Despite nearly identical structural parameters of the two compounds there is a different magnetic ground state. Work supported by DFG and ESF-HFM.

TT 20.26 Wed 14:00 Poster A

Bilayer antiferromagnet with four-spin interaction — •Thomas C. Lang[1] and Anders W. Sandvik[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]Department of Physics, Boston University

We investigate a spin-1/2 Heisenberg antiferromagnet with four-spin interaction on bilayer square and honeycomb lattices. In addition to the standard Neel and quantum disordered phases, these models can be expected to have a valence-bond-solid (VBS) phase. We locate the VBS phase and investigate, in particular, a transition from quantum disorder to VBS. This is potentially a deconfined quantum critical point. We use the recently introduced ground state projection Monte Carlo method in the valence bond basis which allows us to study these models without negative-sign problems.

TT 20.27 Wed 14:00 Poster A

Causes of weak-localization of electrons on liquid helium — •Jürgen Klier, Annie Wakata, and Paul Leiderer — Universität Konstanz, Fachbereich Physik, D-78457 Konstanz

Weak localization (WL) is a quantum effect caused by the coherence among multiple elastic-scattering paths of a conduction electron. This coherence leads to an enhanced backscattering probability and an increase in the resistivity over the classical Drude model. We have investigated the dephasing processes in a weak localization experiment of a two-dimensional electron system on liquid helium. From low-field magnetoconductivity measurements we can separate the damping of WL on the dephasing of electrons due to electron-electron interaction and the motion of the helium vapour atoms. We observe an intermediate regime where both damping mechanisms are of comparable importance and determine the transition from one dominant regime to the other. This is the first observation of a cross-over from the simple exponential decay to the cubic exponential damping in such a system.

TT 20.28 Wed 14:00 Poster A

Anion ordering transition in organic quantum spin chains

$(TMTTF)_2X$ investigated by ESR and SQUID — •Shadi Yasin, Belal Salameh, Michael Dumm, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Germany

The organic charge-transfer salts $(TMTTF)_2X$ are $S = 1/2$ quantum spin chains. The low temperature physical properties of these materials depend strongly on the size and shape of the counter-anion X. Species with non-centrosymmetric anions like ReO_4, BF_4, and SCN show an anion-order transition at 40 K $< T_{AO} <$ 160 K. This breaking of the inversion symmetry of the molecular conductors has strong impact on the spin and charge degrees of freedom. We investigated the nature of the anion-ordered ground state by temperature dependent ESR and SQUID experiments. We found that the temperature dependence of the ESR linewidth and the spin susceptibility changes drastically below T_{AO} in the compounds with $X = ReO_4$ and BF_4 where a spin gap Δ_σ opens in the non-magnetic anion-ordered ground state. Contrary, in $(TMTTF)_2SCN$ the ESR linewidth and the spin susceptibility show only a shallow change below T_{AO}. This is an indication that anion order is accompanied by charge order but not by spin order.

TT 20.29 Wed 14:00 Poster A

Low-temperature study of an $S = 1/2$ antferromagnetic Heisenberg chain close to the field-induced quantum critical point — •K. Remović-Langer[1], Y. Tsui[1], U. Tutsch[1], V. Pashchenko[1], B. Wolf[1], A. V. Prokofiev[2], and M. Lang[1] — [1]Physikalisches Institut, J. W. Goethe-Universität, Frankfurt(M), Germany — [2]Institut für Festkörperphysik, Technische Universität Wien, Wien, Austria

We present magnetic susceptibility, electron spin resonance (ESR), and magnetocaloric effect (MCE) measurements of the compound $[Cu(\mu\text{-}ox)(4\text{-}apy)_2(H_2O)]_n$ [1]. Magnetic susceptibility measurements, performed in the temperature range from 50 mK up to 300 K, can be interpreted within an uniform 1D Heisenberg model with a small antiferromagnetic exchange interaction of $J/k_B \approx (3.14 \pm 0.1)$K. The magnetization $M(B)$ was obtained by integrating the susceptibility data. At the lowest temperatures, $M(B)$ saturates at a field $\mu_0 H_{sat} = (4.3 \pm 0.1)$ T. The angular dependence of the resonance absorption line, obtained from ESR measurements, reveals the magnetic anisotropy of the $S = 1/2$ copper ions. MCE measurements were performed at low temperatures and at fields in the vicinity of the saturation field which, at zero-temperature, marks a quantum phase transition with intriguing magnetocaloric properties[2]. The significance of the MCE results will be discussed.

[1]A. V. Prokofiev et. al. , submitted to Crystal Research and Technology. [2]L. Zhu et. al., Phys. Rev. Lett. **91**, 066404 (2003); M. E. Zhitomirsky, A. Honecker, J. Stat. Mech.: Theor. Exp (2004) P07012.

TT 20.30 Wed 14:00 Poster A

^{7}Li NMR and ESR study of the Cu spin dynamics and Li mobility in the frustrated spin-1/2 chain cuprate Li_2ZrCuO_4 — •Y. Arango[1], E. Vavilova[1,2], V. Kataev[1,2], S.-L. Drechsler[1], A. Moskvin[3], O. Volkova[1,4], A. Vasilyev[4], and B. Büchner[1] — [1]Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany — [2]Kazan Physical Technical Institute of RAS, 420029 Kazan, Russia — [3]Ural State University, 620083 Ekaterinburg, Russia — [4]Moscow State University, 119992 Moscow, Russia

The new frustrated quasi-1D quantum spin system Li_2ZrCuO_4 is close to a ferromagnetic critical point and exhibits unusual thermodynamic properties. The crystal structure of Li_2ZrCuO_4 contains CuO_2 chains and two different types of Li positions. The first type is regularly occupied. The second type is 50 % occupied. Thus, there are two equivalent positions for type II between which the Li ions can hop. We have measured Cu^{2+} ESR and ^{7}Li NMR in Li_2ZrCuO_4. The ESR data reveal a strong enhancement of quasi-static spin correlations below $\sim 50-60$ K and possibly a transition to a magnetically ordered state below ~ 8 K. The ^{7}Li NMR spectrum consists of two lines which can be assigned to the two nonequivalent Li positions. The analysis of the spectral shape and relaxation times T_1 and T_2 strongly corroborates the ESR results regarding the slowing down of the Cu spin dynamics and gives a clear indication of the magnetric order at low T. Moreover, the NMR monitors the mobility of the Li ions in Li_2ZrCuO_4 and yields a characteristic temperature $T_g \sim 80$ K for the quenching of the hopping of the Li ions between the two type II-positions.

TT 20.31 Wed 14:00 Poster A

In_2VO_5 - a new low dimensional S = 1/2 system probed by magnetic resonance — •M. Yehia[1], E. Vavilova[1], T. Taetz[2], A. Möller[2], V. Kataev[1], B. Büchner[1], N. Hollmann[3], and J.A. Mydosh[3] — [1]Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany — [2]Institut für Anorganische Chemie, Universität zu Köln, 50939 Köln, Germany — [3]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

In_2VO_5 contains paramagnetic V^{4+} ($3d^1$, $S = 1/2$) ions. The structural feature is a double chain of VO_6-polyhedra along the b-axis. X-ray diffraction reveals a change of the lattice contraction from isotropic at high T to anisotropic below 150 K. In the spin sector this leads to a change in the spin topology from coupled $S = 1/2$ chains to coupled $S = 1/2$ triangles along the b-axis. ESR and ^{51}V NMR data give evidence that the structural changes have a strong impact on the magnetic properties. The static susceptibility suggests a transition from ferromagnetic exchange above a characteristic temperature $T^* \sim 120$ K to antiferromagnetic (AF) exchange at $T < T^*$. ESR and NMR reveal a slowing of the d-electron spin dynamics as a consequence of enhanced AF correlations at $T < T^*$ and an AF ordering at $\sim$20 K. Remarkably, a well defined ESR signal from V^{4+} ions can only be observed below T^*, strongly suggesting the localization of the d-states. Indeed, the resistivity data, $\rho(T)$, show a dramatic increase of ρ and a transition to an insulating behaviour at $T < T^*$. We discuss these experimental observations in terms of a significant interplay between structure, magnetism and charge mobility in this novel material.

TT 20.32 Wed 14:00 Poster A

Magnetic heat conduction in Ca-doped $SrCuO_2$ spin chains and related systems — Patrick Ribeiro, •Nikolai Hlubek, Anja Waske, Christian Hess, and Bernd Büchner — IFW-Dresden, Helmholzstr.20, 01069 Dresden, Germany

We present new results on the heat conduction of the spin-chain system $Sr_{1-x}Ca_xCuO_2$. The structure of this material contains two parallel antiferromagnetic $S = 1/2$ copper chains with a $J_{||} \approx 2100K$. They are decoupled from each other due to a frustration arising from the displacement of half a Cu-Cu length between them. Additionally to the regular phonon heat conduction, this material possesses spinon contributions in the chain direction. A separation of both contributions is ambiguous, since the spinon contribution appears in form of a hump on the low-temperature phonon peak. By substituting the Sr by the isovalent Ca, we aim at a separation of both contributions. The smaller Ca leads to an increased scattering of phonons and consequently to the suppression of the phonon heat conductivity. Since strong changes of the magnetic properties by this doping are unlikely, we expect the spinon contributions to remain untouched. However, a reduction of the spinon contribution is observed upon doping. To explain this observation two scenarios are considered: on the one hand the spin-phonon-drag effect, on the other a possible Ca-induced modulation of the coupling constant due to the doping, that would lead to spinon scattering. Comparisons with earlier results on similar systems, such as the spin ladder $Sr_{14}Cu_{24}O_{41}$ and the buckled pseudo-two-leg spin ladder $CaCu_2O_3$, are carried out.

TT 20.33 Wed 14:00 Poster A

Electrochemical doping of Vanadium Oxide Nanotubes — •A. Popa[1], I. Hellmann[1], R. Klingeler[1], V. Kataev[1], E. Vavilova[1,2], Y. Arango[1], C. Täschner[1], X. Liu[1], M. Knupfer[1], C. Masquelier[3], and B. Büchner[1] — [1]Leibniz-Institute for Solid State and Materials Research IFW Dresden, Dresden, Germany — [2]Kazan Physical Technical Institute, RAS, Kazan, Russia — [3]Laboratoire de Réactivité et de Chimie des Solides, Amiens, France

Vanadium oxide nanotubes (VOx-NTs) exhibit diverse properties ranging from spin frustration and semiconductivity to ferromagnetism by doping with either electrons or holes [1]. We have applied optical, photoemission and EELS as well as static magnetization, ESR and NMR studies in order to obtain insight into the rich physics of these materials. Our data suggest an averaged vanadium valency of about 4.4+ in the undoped case [2]. We observe two magnetically nonequivalent vanadium sites, attributed to V^{4+} ions ($3d^1, S = 1/2$) in octahedral and tetrahedral oxygen coordination and there are strong indications that antiferromagnetic dimers and trimers occur in the vanadium-spin chains in the walls. We find a spin gap of the order of 700 K [3]. Upon electron doping of VOx-NTs, our spectroscopic data confirm a higher number of magnetic V^{4+} sites. Besides, the magnetic response was studied after the electrochemical insertion of lithium. For certain doping levels, a ferromagnetic signal at room temperature was found.

[1] L. Krusin-Elbaum *et al.*, Nature **431**, 672 (2004)
[2] X. Liu *et al.*, Phys. Rev. B **72**, 115407 (2005)
[3] E. Vavilova *et al.*, Phys Rev. B **73**, 144417 (2006)

TT 20.34 Wed 14:00 Poster A

Magnetic exchange interactions in 1D and 2D cuprates — Ulrike Nitzsche[1], Stefan-Ludwig Drechsler[1], and •Helge Rosner[2] — [1]IFW Dresden — [2]MPI CPfS Dresden

In many copper oxygen networks, especially for Cu-O bond angles close to 90°, ferromagnetic (FM) interactions play an important role in addition to the well known superexchange $J \sim t^2/U$. We present a systematic study of the electronic structure and the exchange integrals J for different types of 1D and 2D spin 1/2 cuprates: edge shared (Li_2CuO_2) and corner shared (A_2CuO_3 [A=Sr,Ca]) single-chains, double-chains ($SrCuO_2$), and planar ($CaCuO_2$, $Sr_2CuO_2Cl_2$, R_2CuO_4 [R=La,Nd,Sm]) arrangements. Based on full potential LDA and LDA+U band structure calculations and subsequent tight-binding (TB) models we estimate sign and magnitude of the most relevant J's. We compare the results of total energy calculations with those of TB models from one-band and multi-band approaches. The FM contributions can be estimated from the difference between the TB and the total energy results. We investigate the effect of the inter-plaquette geometry (edge shared vs. corner shared CuO_2 plaquettes) and the intra-plaquette geometry under pressure on the coupling strength. In excellent agreement with various experiments, our calculations result in: (i) dominant FM nearest neighbor (NN) coupling $J_1 \sim$ -17 meV in Li_2CuO_2, (ii) strongly enhanced AFM NN $J_1 \sim$ 180 meV for the 1D corner shared chains compared to (iii) $J_1 \sim$ 110...150 meV for the 2D compounds where we observe a sequence of J's (with respect to the cations) in agreement with the experimental data.

TT 20.35 Wed 14:00 Poster A

Anisotropy of superconducting critical fields of α-(BEDT-TTF)$_2$KHg(SCN)$_4$ under pressure — •Sebastian Jakob, Karl Neumaier, Werner Biberacher, and Mark Kartsovnik — Walther-Meissner-Institut, Garching, Germany

Our previous studies of the "magnetic field - pressure - temperature"phase diagram of the layered organic conductor α-(BEDT-TTF)$_2$KHg(SCN)$_4$ have revealed an interesting interplay between a charge density wave (CDW) and a superconducting (SC) state [1]. At a critical pressure of 2.5 kbar the CDW state is completely suppressed and a sharp transition into a SC state is observed below 100 mK. For pressures below 2.5 kbar there is a coexistence of the superconducting and CDW state, but this is likely a spatially inhomogenous state. The neighbouring of a CDW and SC state is an interesting situation and rises questions about the nature of the superconductivity. We have therefore investigated the anisotropy of the critical fields at a pressure slightly above the critical one. The experiments were performed in a dilution refrigerator down to 25 mK. Two-axes rotation of the magnetic field allowed the exact determination of the anisotropy parallel and perpendicular to the layers, but also the inplane anisotropy.

[1] D. Andres, M. V. Kartsovnik, W. Biberacher, K. Neumaier, E. Schuberth, H. Müller, Phys. Rev. **B 72**, 174513 (2005).

TT 20.36 Wed 14:00 Poster A

ESR investigations of the phase diagram of 2-dim organic conductors in the vicinity of the Mott-Hubbard transition — •Shadi Yasin, Michael Dumm, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

In the two-dimensional layered organic charge-transfer salts κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br$_x$Cl$_{1-x}$, it is possible to tune the electronic and magnetic properties by bandwidth control, i. e., by a systematic variation of the external or chemical pressure (anion size) as presented here. While the materials with low Br content x are antiferromagnetic insulators at low temperatures, the materials with high Br concentration show superconductivity. We studied the phase diagram in the vicinity of the Mott-Hubbard transition as a function of Br content by electron-spin resonance in the temperature range 4.2 K $< T <$ 295 K along all three crystal axes. A detailed analysis of the ESR linewidth, the spin susceptibility and the microwave conductivity which was derived from the asymmetric Dysonian shape of the absorption lines was performed. These results enabled us to map the critical temperatures of the metal-to-insulator, antiferromagnetic and superconducting transitions for different Br dopings. We will also discuss the unconventional behaviour of ESR linewidth and spin susceptibility at temperatures below 50 K where the properties of the materials are dominated by strong electronic correlations.

TT 20.37 Wed 14:00 Poster A

Probing the metal-insulator transition in $\kappa-(ET)_2Cu_2(CN)_3$ by hydrostatic He-gas pressure experiments — Christian Strack[1], Michael Lang[1], and •John Schlueter[2] — [1]Physikalisches Institut, J.W.-Goethe-Universität, Frankfurt/Main, FOR 412 — [2]Materials Science Division, Argonne NL, Illinois, USA

The title compound has gained considerable interest from both the theoretical and experimental side, see e.g. [1+2]. It is a Mott-insulator characterized by a triangular lattice with almost perfect magnetic frustration. This leads to the absence of long-range magnetic ordering down to 32 mK, the lowest temperature investigated so far [3]. The system, therefore, is a promising candidate for a quantum spin liquid without symmetry breaking [4], which contrasts with the $\kappa-(ET)2Cu[N(CN)2]Cl$ salts, where a less strong frustration gives rise to long-range magnetic order of local moments. Both systems become metallic and superconducting under pressure with a similar resistivity profile. Comparative studies of the pressure-induced insulator to metal transition for both compounds thus provide a deep insight into the nature of the correlated electron system and, specifically, the role of magnetism. Using both temperature-dependent resistivity measurements under pressure and pressure sweeps at constant temperatures, the phase diagram of the title compound has been explored. A detailed study of the transition from insulator to metal will be presented.

[1] S. Lee et al. PRL 95, 036403 (2005) [2] E. Ohmichi et al. PRB, Vol. 57, No. 13 [3] Y. Shimizu et al. PRL, Vol. 91,No. 10 (2003) [4] Y. Kurosaki et al. PRB, 95,177001 (2005)

TT 20.38 Wed 14:00 Poster A

Spin liquid ground state in the frustrated $S = 1/2$ square lattice compound $PbVO_3$ — Alexander Tsirlin[1,2], Roman Shpanchenko[2], Evgeny Antipov[2], Alexei Belik[3], Eiji Takayama-Muromachi[3], and •Helge Rosner[1] — [1]MPI CPfS, Dresden, Germany — [2]Department of Chemistry, MSU, Russia — [3]NIMS, Tsukuba, Japan

The $S = 1/2$ square lattice is known to be one of the simplest models of low-dimensional spin systems depicting the magnetic properties of many transition metal compounds like La_2CuO_4. If one considers nearest-neighbor (NN) interactions only, long-range spin order is established in the square lattice. Nevertheless, taking into account next-nearest neighbor (NNN) interactions may result in strong frustration of the spin system and give rise to unusual collinear magnetic order or spin liquid ground states. Here, we present a joint experimental and computational study of a novel layered vanadium oxide $PbVO_3$ realizing a square lattice of magnetic V^{+4} atoms. Our results show that in $PbVO_3$ antiferromagnetic NN (J_1) as well as NNN (J_2) interactions are present. The J_2/J_1 ratio is about 0.3 corresponding to a boundary between AFM ordered and spin liquid ground states. This conclusion is in a perfect agreement with magnetic susceptibility and specific heat measurements showing no sign of long-range spin order down to 2 K. $PbVO_3$ is likely to be the first system showing spin liquid ground state for the frustrated $S = 1/2$ square lattice.

The Alfred Toepfer Foundation and the Emmy-Noether program are acknowledged for financial support.

TT 20.39 Wed 14:00 Poster A

Initial stages of growth of the strongly correlated Fe_3O_4 thin films — •Stefan Klein[1], Chun Fu Chang[1], Zhiwei Hu[1], Philipp Hansmann[1], Hong-Ji Lin[2], Chien-Te Chen[2], and Liu Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]National Synchrotron Radiation Research Center,101 Hsin-Ann Road, Hsinchu 30076, Taiwan

We have investigated the initial stages of growth of the polar Fe_3O_4(001) thin films using reflection high-energy electron diffraction, low-energy electron diffraction and soft X-ray absorption spectroscopy (XAS). A series of epitaxial thin films with varying thicknesses were grown by molecular-beam epitaxy in O_2 atmosphere on MgO(001) substrates. From the analysis of the XAS spectra, we established a model for the growth process. Furthermore, the surface reconstruction of Fe_3O_4(001) will also be discussed. Supported by the DFG through SFB 608.

TT 20.40 Wed 14:00 Poster A

X-ray absorption and photoemission study of spin state and metal-insulator transition in$GdBaCo_2O_{5.47}$ — •Z. Hu[1], Hua Wu[1], T. Koethe[1], M. W. Haverkort[1], T. Burnus[1], J. Gegner[1], C. Zobel[1], T. Lorenz[1], S. N. Barilo[2], H.-J. Lin[3], N. B. Brookes[4], C. T. Chen[3], and L. H. Tjeng[1] — [1]II. Physikalisches Institut,Universität zu Köln, Zülpicher Straße 77, 50937 Köln — [2]Institute of Solid State and SemiconductorsPhysics, National Academy of Sciences, Belarus — [3]National Synchrotron RadiationResearch Center, Taiwan —

[4]European Synchrotron Radiation Facility, France

The fundamental physics of the magnetoresistance materials $R\mathrm{BaCo_2O_{5.5}}$ (R =Sm, Eu, Gd, Tb, Dy, Y), particularly the issue of spin-state and metal-insulator transition (MIT), is currently under intense debate. Using valence-band photoemission spectra and x-ray absorption spectra at both the O-K and Co-$L_{2,3}$ edges, we found that crossing the MIT, the band gap decreases but does not collapse across the MIT. More significantly, our spectroscopic evidence firmly rules out the widely accepted model for the low-temperate phase, namely that the Co^{3+} ions in the octahedral sites are mainly low spin and in the pyramidal sites intermediate spin. We rather found that the MIT in this system is very similar to the high temperature (600 K) MIT of $LaCoO_3$.

TT 20.41 Wed 14:00 Poster A

Spectral line shapes in soft x-ray diffraction — •C. Schüßler-Langeheine, J. Schlappa, M. W. Haverkort, and L. H. Tjeng — II. Physikalisches Institut, Universität zu Köln

Resonant diffraction in the soft x-ray range is a powerful spectroscopic method to study order phenomena like charge, spin and orbital order as they are found in correlated electron systems. In particular this technique is capable to differentiate between true modulations of the electronic states and pure modulations of the lattice like strain waves. For energetically sharp resonances like the $L_{2,3}$ thresholds of transition metals, the spectral shape of the diffraction spectrum differs significantly between a predominantly structural and a predominantly electronic superstructure. This difference is caused by the interference of resonant and non-resonant scattering, which acts differently in the two cases and can be used as a qualitative fingerprint of the two scenarios. Supported by the DFG through SFB 608.

TT 20.42 Wed 14:00 Poster A

Coulomb correlations in Cu_2O and ZnO: Importance of both transition-metal U_{dd} and Oxygen U_{pp} — •Sven Binder, Hua Wu, Thomas Koethe, Stefan Klein, and Liu Hao Tjeng — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln

Standard local density approximation (LDA) band structure calculations for Cu_2O and ZnO produce valence band spectra which show significant deviations from the experimentally observed spectra as obtained from photoemission. This is surprising since one may assume that Coulomb interactions can be well taken into account in a mean-field manner for closed shell systems. In an attempt to resolve this issue, we have performed LDA+U calculations. We have discovered that not only we have to include the Coulomb interaction in the 3d shell (U_{dd}) but also in the O 2p shell (U_{pp}). To justify this approach, we have set out to determine experimentally the values for U_{dd} and U_{pp} by performing L_3VV and KLL Auger spectroscopies for Cu_2O and ZnO.

TT 20.43 Wed 14:00 Poster A

Magnetic and electrical properties of EuC_2 — •Oliver Heyer[1], Derk Wandner[2], Nils Hollmann[1], Uwe Ruschewitz[2], John Mydosh[1], Axel Freimuth[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, D-50937 Köln — [2]Institut für Anorganische Chemie, Universität zu Köln, D-50939 Köln

We present measurements of the magnetization M, the specific heat c_p and the resistance ρ of EuC_2.This compound is interesting because Eu exists in the oxidation states +2 as well as +3. Thus EuC_2 may be located between the pure ionic carbides of the divalent alkaline earth (CaC_2, SrC_2) and the metallic carbides of the trivalent lanthanides (LaC_2, CeC_2). Possibly, one may even change the valency under pressure or temperature variation. The magnetization and the specific heat data indicate a ferromagnetic ordering at $T_\mathrm{c} \sim 12\,\mathrm{K}$. According to a very small hysteresis EuC_2 may be classified as a soft ferromagnet. Above T_c the resistance shows a semiconducting behaviour. With the onset of the magnetic order the resistance decreases over 4 orders of magnitude indicating a metal-insulator transition (MIT). Moreover, an applied magnetic field shifts the MIT temperature to higher values, resulting in a colossal magnetoresistance with changes in the resistivity up to 6 orders of magnitude. This behaviour strongly resembles the colossal magnetoresistance of the better-known system of Eu-rich EuO.

TT 20.44 Wed 14:00 Poster A

Crystal growth, dielectric and magnetic investigation of 3d transition metal tungstates $M\mathrm{WO_4}$ (M = Mn, Fe, Co, Ni) — •Sven Jodlauk[1], Daniel Khomskii[2], Petra Becker[1], Ladislav Bohatý[1], Oliver Heyer[2], Nils Hollmann[2], Harald Kierspel[2], Thomas Lorenz[2], and John Mydosh[2] — [1]Institut für Kristallographie, Universität zu Köln — [2]II. Physikalisches Institut, Universität zu Köln

Some tungstates $M\mathrm{WO_4}$ seem to be promising candidates for multiferroics whose dielectric properties are caused by a spiral spin ordering. Single-crystal growth of 3d transition metal tungstates $M\mathrm{WO_4}$ (M = Mn, Fe, Co, Ni) can either be done using the flux technique and an adapted melt solvent from the system Na_2WO_4 - WO_3 (basing on early work of Schultze et al. [1]) or, especially in the case of $MnWO_4$, from high-temperature melt. This latter method is able to prevent Mn^{2+} from oxidation. Single crystals of $MnWO_4$ obtained from our crystal growth are of ruby-red color and of dimensions up to 25 * 5 * 4 $\mathrm{mm^3}$. Temperature dependent dielectric and pyroelectric measurements on $MnWO_4$ (using a (010) plate) reveal anomalies which correlate with the anomalies that were detected for temperature dependent magnetic susceptibility. This signals that $MnWO_4$ is a magneto-electric multiferroic. Results of this work have been published in [2].

References

[1] D. Schultze, K.-Th. Wilke, Ch. Waligora: Z. anorg. allg. Chemie **352** (1967) 184-191. [2] O. Heyer *et al.*: J. Phys.: Condens. Matter **18** (2006) L471-L475.

TT 20.45 Wed 14:00 Poster A

Structural and magnetic dimers in the spin-gapped system $\mathrm{CuTe_2O_5}$ — •Hans-Albrecht Krug von Nidda[1], Joachim Deisenhofer[2], Rushana Eremina[1,3], Tatiana Gavrilova[3], Mike Whangbo[4], and Alois Loidl[1] — [1]Experimental Physics V, Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany — [2]Département de Physique de la Matière Condensée, Université de Genève, CH-1211 Genève 4, Switzerland — [3]E. K. Zavoisky Physical-Technical Institute, 420029 Kazan, Russia — [4]Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204, USA

We investigate the magnetic properties of the system $CuTe_2O_5$ by susceptibility and electron spin resonance ESR measurements. The anisotropy of the effective g-factors and the ESR linewidth indicates that the anticipated structural dimer does not correspond to the singlet-forming magnetic dimer. Moreover, the spin susceptibility of $CuTe_2O_5$ can only be described by taking into account interdimer interactions of the same order of magnitude than the intradimer coupling. Analyzing the exchange couplings in the system we identify the strongest magnetic coupling between two Cu ions to be mediated by a super-superexchange interaction via a bridging Te ligand, while the superexchange coupling between the Cu ions of the structural dimer only results in the second strongest coupling.

TT 20.46 Wed 14:00 Poster A

Electric transport properties of $\mathrm{LaAlO_3/SrTiO_3}$ interfaces studied by scanning electron microscopy — •Christian Gürlich[1], Matthias Ruoff[1], Stefan Thiel[2], Christof Schneider[2], German Hammerl[2], Christoph Richter[2], Jochen Mannhart[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut, Experimentalphysik II, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — [2]Center for Electronic Correlations and Mangnetism, Institut of Physics, Augsburg University, D-86135 Augsburg, Germany

It was shown recently that conducting electron gases are formed at interfaces in heterostructures consisting of insulating oxides such as $SrTiO_3/LaTiO_3$ (STO/LTO) or $LaAlO_3/SrTiO_3$ (LAO/STO) [1]. These conducting electron gases might be confined to sheets that are only very few nanometers thick. Lateral confinement into a bridge-like structure has been realized for STO/LAO interfaces, using lithographic patterning by modulating the thickness of the LAO layers with unit cell resolution [2]. Here, we present a scanning electron microscopy study of the electric transport properties of such structures. Irradiation with a focused electron beam induces pronounced changes of the sample resistance, with a typical reduction by more than a factor of two at 300 K. After switching off the electron beam, the resistance returns to the initial state with relaxation times above several hundred seconds.

[1] H. Y. Hwang, Science vol. 313, 1895 (2006) and references therein.
[2] C. W. Schneider *et al.*, Appl. Phys. Lett. vol. 89, 122101 (2006).

TT 20.47 Wed 14:00 Poster A

Unoccupied electronic structure of TiOCl studied by XAS — •Sebastian Glawion[1], Götz Berner[1], Matthias Schlachter[1], Michael Sing[1], Markus Hoinkis[2], Gianina Gavrila[3], Leonardo Pisani[4], Roser Valenti[4], and Ralph Claessen[1] — [1]Experimentelle Physik 4 and Röntgen Research Center for Complex Materials, Universität Würzburg, D-97074 Würzburg, Germany — [2]Experimentalphysik II, Universität Augsburg, D-86135 Augsburg, Germany — [3]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [4]Institut für Theoretische Physik, Universität Frankfurt, D-60054 Frankfurt, Germany

TiOCl is a Mott-insulating quantum magnet showing a dimerized spin-Peierls phase for temperatures below T_c1=67K. This phase is reached through two distinct phase transitions. The intermediate phase shows incommensurate order, while the susceptibility of the high-T phase nicely reflects the behaviour of a 1D Heisenberg antiferromagnet. Intensive studies in this latter phase have been conducted on the occupied density of states in the valence band both by (AR)PES and various calculations. However, since the low-T phase cannot be reached by PES due to charging problems, we conducted X-ray absorption studies searching for possible changes in the electronic structure induced by the different kinds of ordering. Our results nicely agree with previous LDA+U and GGA+U calculations but do not seem to show major differences between the different phases.

TT 20.48 Wed 14:00 Poster A

Electronic Raman scattering and phonon anomalies in Na_xCoO_2. — Vladimir Gnezdilov[1], Patric Scheib[2], •Peter Lemmens[2], Fangcheng Chou[4], Lambert Alff[5], Yoshiharu Krockenberger[3], Hanns-Ulrich Habermeier[3], Chengtian Lin[3], and Bernhard Keimer[3] — [1]Institute for Low Temperature Physics and Engineering, NASU, Kharkov, Ukraine — [2]Institut für Physik der kondensierten Materie, TU Braunschweig, Braunschweig — [3]Max-Planck-Institute for Solid State Research, Stuttgart — [4]Center for Materials Science and Engineering, MIT, Cambridge, USA — [5]Institute of Material Science, TU Darmstadt, Darmstadt

Raman scattering in nonsuperconducting and superconducting cobaltates $Na_xCoO_2 \cdot yH_2O$ shows pronounced anomalies in the phonon as well as the electronic contribution to the scattering cross section. The effect of doping and hydration on these anomalies is studied and used for a characterization of single crystals and thin films. Work supported by DFG, ESF-HFM and MRSEC Program of NSF under award number DMR 02-13282.

TT 20.49 Wed 14:00 Poster A

Low-Temperature Antiferromagnetic Phase Transition in α-YbPdSn — •Tobias Görlach[1], Sergiy Putselyk[1], Andreas Hamann[1], Tihomir Tomanic[1], Falko Schappacher[2], Rainer Pöttgen[2], and Hilbert v. Löhneysen[1,3] — [1]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany — [2]Institut für Anorganische und Analytische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstr. 30, D-48149 Münster, Germany — [3]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany

Ternary intermetallic compounds of the type YbTX where T is a transition metal and X is a main group metal, show a wide variety of magnetic properties at low temperatures [1]. More specifically, stannides (X = Sn) show different types of magnetic order. While YbNiSn orders ferromagnetically at T_C = 5.6 K, YbRhSn and YbPtSn order antiferromagnetically at 1.85 K and 3.5 K, respectively, YbPtSn also being metamagnetic. Here we present evidence for magnetic order at very low temperatures in YbPdSn, whose magnetic properties have previously been investigated at temperatures above 4.2 K only. Our low-temperature measurements of the specific heat and the magnetic susceptibility indicate an antiferromagnetic phase transition at 200 mK which is suppressed rapidly in moderate magnetic fields.

[1] R. Pöttgen, D. Johrendt and D. Kußmann, in: *Handbook of the Physics and Chemistry of the Rare Earths* (Elsevier Science B.V., Amsterdam, 2001), vol. **32**, ch. 207, pp. 455–515.

TT 20.50 Wed 14:00 Poster A

Thermal expansion and specific heat of magnetically frustrated $(Ni_{1-x}Co_x)_3V_2O_8$ — •Qin Zhang[1], William Knafo[1,2], Kai Grube[1], Hilbert v. Löhneysen[1,2], Christoph Meingast[1], and Thomas Wolf[1] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany

$Ni_3V_2O_8$ and $Co_3V_2O_8$ both have the same basic kagome-staircase structure, leading to geometric frustration of the magnetic ordering of the spins on Ni and Co sites. Both compounds exhibit a number of magnetic phase transitions at low temperatures, which partially relieve the frustration. In addition to magnetic ordering, these compounds also exhibit ferroelectric properties. Here we present thermal expansion and specific heat data on high-quality single crystals of $(Ni_{1-x}Co_x)_3V_2O_8$, which allow us to map out the phase diagram of the Ni-Co series, as well as to calculate various pressure derivatives associated with magnetic ordering.

TT 20.51 Wed 14:00 Poster A

Magnetisation of ferromagnetic Pr_5Si_3 under hydrostatic pressure — •Stefan Legl[1], Christian Pfleiderer[1], Dmitri Souptel[2], and Günter Behr[2] — [1]Physik Department E21, Technische Universität München, D-85748 Garching, Germany — [2]IFW Dresden, PF 270116, D-01171 Dresden, Germany

We report the low temperature magnetisation, specific heat and resistivity of single crystal Pr_5Si_3 at ambient pressure under magnetic field up to 9T and temperatures down to 3K.

Pr_5Si_3 orders ferromagnetically below T_c=50K. The ferromagnetic state is strongly anisotropic where the basal plane in the hexagonal crystal structure is the easy magnetic plane.

Under hydrostatic pressures up to 18 kbar the magnetisation for temperatures down to 3K and magnetic fields up to 9T shows only a weak variation of the ordered moment and T_c. Magnetisation loops at low magnetic fields show changes characteristic of the emergence of a magnetic modulation under pressure.

TT 20.52 Wed 14:00 Poster A

Transport and Ordering of Polarons in PrCaMnO: Electric induced Colossal Resistance Effect — •Sebastian Schramm, Peter Moschkau, Jörg Hoffmann, and Christian Jooss — Institut für Materialphysik, Universität Göttingen

The resistivity of the low-bandwidth manganite $Pr_{1-x}Ca_xMnO_3$ (x = 0.3 and x = 0.5) is affected by electric fields and currents. This Colossal Electroresistance (CER) includes a continuous lowering of the resistivity for high temperatures with increasing current and a sharp resistivity-drop at the characteristic temperature T_c for high currents. In thin films of PrCaMnO prepared by Pulsed Laser Deposition on $SrTiO_3$-substrates the resistivity in a wide temperature range can be described by a model, where thermally activated polarons (TAP) are the effective charge carriers. In a detailed series the resistivity especially of annealed samples shows a good agreement with the TAP-model. The change of resistivity in the PrCaMnO-films is a current-induced effect, strong Joule heating occurs as a secondary effect due to inherent nonlinearities in the current-voltage-characteristics. The resistivity-drop is accompanied by the destruction of a polaron-ordered phase and by a related structural modification of the lattice. The starting point of this dynamical disordering process is defined by a temperature dependent critical current and a critical electric field.

TT 20.53 Wed 14:00 Poster A

Development of an array of calorimetric low temperature detectors for heavy ions — •A. Echler[1,2], V. Adrianov[1,2], A. Bleile[1,2], P. Egelhof[1,2], S. Ilieva[1,2], O. Kiselev[1], S. Kraft-Bermuth[1,2], and J. P. Meier[1,2] — [1]Gesellschaft für Schwerionenforschung, Darmstadt, Germany — [2]Johannes Gutenberg Universität Mainz, Germany

Calorimetric low temperature detectors (CLTDs) for heavy-ion detection have been frequently demonstrated to achieve an excellent relative energy resolution of $\Delta E/E$ = 1-5×10^{-3} in a wide range of ions and energies. Such detectors were already successfully applied in accelerator mass spectrometry, and have the potential to be applied in superheavy element research where CLTDs as high resolution energy detectors combined with time-of-flight detectors may be used for identification of superheavy nuclei with Z $\geq$ 113. The CLTDs developed up to now have an active area of approximately 3×3 mm^2, not sufficient to fully exploit their potential. To increase the active area, an array of CLTDs for heavy ion research is currently subject of design and investigation. As a first step, a 4×2 pixel prototype array with eight individually temperature controlled pixels and a total active area of 12×6 mm^2 was realized and its performance under heavy ion irradiation was investigated. Results from a recent experiment performed with 4.8 MeV/u ^{132}Xe-ions will be presented, and future perspectives will be discussed.

TT 20.54 Wed 14:00 Poster A

Orbital responses in $3d^1$ perovskite titanates — •Luis Craco — Max-Planck Institute for Chemical Physics of Solids, Noethnitzer Str. 40, D-01187 Dresden, Germany

$LaTiO_3$ and $YTiO_3$ have long been considered as classic examples of systems where the change of electron correlations originates form a change in the $3d$ electron hopping, which is governed by the Ti-O bond angles. Using a combination of ab initio and correlated many-body treatments, we consider the role of lattice distortions and multi-orbital electron interactions in these classical $3d^1$ perovskites. We show how the Mott-Hubbard insulating state is affected by structural distortions and the concomitant orbital polarization pattern. For this we use the LDA+DMFT method, which combines the real one-electron band structure with dynamical effects of strong, electron interactions. Our band-structure results are consistent with a removal of the t_{2g} and e_g orbital degeneracy due to orthorhombic distortions. In this real band-structure, we show that the Mott insulating state is driven by strong electron interactions. The obtained correlated spectra shows good agreement with experiments (photo-emission and/or optics). We find that $La(Y)TiO_3$ are described as orbitally non-degenerate systems, where multi-orbital correlations, orbital polarization and disorder are very important in determining the nature of the paramagnetic insulating state. As an extension of our work, we plan to describe the (ferromagnetic) ground-state properties of $YTiO_3$ and the effect of pressure in the system.

TT 20.55 Wed 14:00 Poster A

Embedding procedure for ab-initio correlation calculations in group II metals — Elena Voloshina, Nicola Gaston, and •Beate Paulus — MPI fuer Physik komplexer Systeme, Noethnitzer Str. 38, 01187 Dresden, Germany

Up to now wavefunction-based ab-initio correlation treatements are possible for semiconductors and insulators applying the method of increments [1]. This method corresponds to a many-body expansion of the correlation energy of the solid in terms of localized entities. A generalization is possible for metals, where two major problems have to be faced: First, a straight-forward localization of the orbitals is not possible, localized entities have to be generated via an embedding scheme. Second is the difference between bulk metals and metal clusters. Within an infinite metal there is a homogeneous distribution of the conduction electrons, whereas in a cluster the charge will move to the surface. In order to apply local wavefunction-based correlation methods to metals using finite fragments of the solid, it is necessary to construct an embedding for these finite entities in such a way that the metallic character is simulated properly. For this purpose we suggest an embedding which has itself no metallic character but can mimic the metal in the internal region, where the atoms are correlated. Here we present different ways to construct such an embedding and discuss the influence of the embedding on the correlation energy of the solid.

[1] B. Paulus, Phys. Rep. 428, 1 (2006).

TT 20.56 Wed 14:00 Poster A

Mean-field theory of quadrupolar ordering in $YbRu_2Si_2$ — •Tetsuya Takimoto and Peter Thalmeier — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

We study theoretically quadrupolar ordering in $YbRu_2Si_2$. At first, we construct an effective Hamiltonian with two Kramers doublets, which consists of CEF, Zeeman, and inter-site interaction terms. In the inter-site term, there are interactions between multipoles which are classified according to the irreducible representations of the point group. Applying mean-field theory, we calculate the H-T phase diagram, order parameters, and the magnetic susceptibility. Comparing our results with experimental data, we identify the type of quadrupolar ordering observed in $YbRu_2Si_2$ as ferro-ordering of quadrupole O_2^2.

TT 20.57 Wed 14:00 Poster A

Realistic description of TTF-TCNQ using massively parallel exact diagonalization — •Andreas Dolfen and Erik Koch — Institut für Festkörperforschung, Forschungszentrum Jülich, Germany

The photoemission spectrum of the quasi one-dimensional organic metal TTF-TCNQ can be described qualitatively using a t-U Hubbard model. For such calculations we have developed a parallel Lanczos code which runs efficiently on modern massively parallel supercomputers like JUBL, Jülich's new BlueGene/L system. To overcome the limitations of the finite system-size we employ cluster perturbation theory (CPT), giving us access to the angular-resolved spectral function with high resolution. As a result, we can resolve the spin-charge separation. Moreover, we compute the total energy of the system by using the Galitskii-Migdal theorem.

Experiments and theoretical estimates for TTF-TCNQ suggest a value for the hopping parameter t. The parameter needed to fit the experiment is, however, larger by a factor of two. We resolve this problem by including realistic values for the next-neighbor interaction V into the model. The effect of this longer-range Coulomb interaction is to broaden the spectrum – very similar to increasing the value of t. This explains why the ad-hoc doubling of t yields a good comparison with experiment. Moreover, we find that the effect of V can be understood already in first-order perturbation theory.

TT 20.58 Wed 14:00 Poster A

Antiferromagnetism and Anderson localization of correlated lattice fermions with disorder — •Krzysztof Byczuk[1], Walter Hofstetter[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Institut fur Theoretische Physik, Johann Wolfgang Goethe-Universitaet, 60438 Frankfurt/Main, Germany

The phase diagram of correlated, disordered lattice fermions is determined within dynamical mean–field theory supplemented by the geometrically averaged ("typical") local density of states. Antiferromagnetic insulator, Mott insulator and Anderson insulator phases are found to be separated by continuous phase transitions. Predictions for cold fermionic atoms on optical lattices and solid state systems are presented.

TT 20.59 Wed 14:00 Poster A

Local moment approach as an impurity solver of multi-orbital dynamical mean-field theory for correlated electrons — Anna Kauch[1] and •Krzysztof Byczuk[2,1] — [1]Institute of Theoretical Physics, Warsaw University, ul. Hoza 69, PL-00-681 Warszawa, Poland — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany

A modified local moment approach is developed, and is applied as an impurity solver of the dynamical mean-field equations for the multiorbital Hubbard model. Assuming the existence of local moments their values are determined through a variational principle by minimizing the corresponding ground state energy. The method is applied to study the Mott metal-insulator transition in the multi-orbital Hubbard model.

[1] A. Kauch and K. Byczuk, Physica B 378-380, 297 (2006). [2] A. Kauch and K. Byczuk, Proceedings of Leschouches summer school, to be published (2007). [3] D. Logan, M.P. Eastwood and M.A. Tusch, J. Phys. Cond. Matter 10, 2673 (1998).

TT 20.60 Wed 14:00 Poster A

Effect of disorder on ferromagnetism in the periodic Anderson model within dynamical mean-field theory — •Unjong Yu, Krzysztof Byczuk, and Dieter Vollhardt — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany

Dynamical mean-field theory (DMFT) has been successfully applied to study of magnetism in strongly correlated systems, especially the Hubbard model [1] and the periodic Anderson model (PAM) [2]. DMFT was also shown to be an adequate tool to investigate the effect of disorder on magnetism in the Hubbard model [3]. In this presentation, we examine the stability of ferromagnetism in the PAM in the presence of binary alloy disorder by using the DMFT together with the quantum Monte-Carlo method. The magnetic phase diagram of the PAM as a function of disorder strength and alloy concentration as well as a carrier density is discussed.

[1] D. Vollhardt, N. Blümer, K. Held, M. Kollar, J. Schlipf, M. Ulmke, and J. Wahle, Advances in Solid State Physics **38**, 383 (1999).

[2] A. N. Tahvildar-Zadeh, M. Jarrell, and J. K. Freericks, Phys. Rev. B **55**, R3332 (1997).

[3] K. Byczuk, M. Ulmke, and D. Vollhardt, Phys. Rev. Lett. **90**, 196403 (2003).

TT 20.61 Wed 14:00 Poster A

Inhomogenous Hubbard model for solids and optical traps — •Rolf Helmes, Luis Craco, and Achim Rosch — Institute of Theoretical Physics, University of Cologne, Zülpicher Str. 77, 50937 Cologne

Inhomogenous systems described by the Hubbard model occur in several very interesting fields of physics: e.g., phase separation and the physcis of domain walls control the properties of manganites, see e.g. [1]. We therefore study domain walls between different phases of the Hubbard model. The interplay of domain walls and their energetics on the one hand and of long-range Coulomb interaction on the other hand, control for example the physics of phase-separation close to a first-order metal-insulator transition. Another example of an inhomogenous Hubbard-model system are fermions in an optical lattice. Here parameters can be tuned such that an "Mott-insulating onion shell" separates two metallic regions in a 3D-trap. We use a generalization of dynamical mean field theory (DMFT) to treat these inhomogeneous correlated systems.

[1] Cheong et al., Nature 2002, 416(6880),518-521

TT 20.62 Wed 14:00 Poster A

Metal-to-insulator transitions in the two-plane Hubbard model — •David Heilmann — (dann:) Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich — (noch:) Phys. Institut der Universität Bonn, Nussallee 12, 53115 Bonn

The question if a Mott insulator and a band insulator are fundamentally different has been the matter of intensive research recently. Here we consider a simple model which allows by tuning one parameter to go continously from a Mott insulator to band insulator. The model consists of two Hubbard systems connected by single particle hopping. The Hubbard Hamiltonian is solved by the Dynamical Mean-Field theory using Quantum Monte Carlo. The quasiparticle spectral function, the opticall conductivity and the self-energy is calculated. Here we particularly focus on the Drude weight.

TT 20.63 Wed 14:00 Poster A

Magnetic properties of correlated electrons coupled to localized spins — •Robert Peters and Thomas Pruschke — Institut für theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

We calculated the magnetic phase diagram of a correlated band coupled to localized spins at each lattice site. This model can be used for d-electrons in cristalline fields where the lower subbands are partially filled and form a local spin which couples to itinerant and interacting electrons. The method we use is the Dynamical Mean Field theory with the Numerical Renormalization group as impurity solver. We observe antiferromagnetism as well as ferromagnetism. We also discuss the behaviour of the MIT at half-filling.

TT 20.64 Wed 14:00 Poster A

Sum rules and vertex corrections for electron-phonon interaction — •Oliver Rösch[1,2], Giorgio Sangiovanni[1], and Olle Gunnarsson[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]Institut für Theoretische Physik, Universität zu Köln

We derive sum rules for the phonon self-energy and the electron-phonon contribution to the electron self-energy of the Holstein-Hubbard model in the limit of large Coulomb interaction U. Their relevance for finite U is investigated using exact diagonalization and dynamical mean-field theory. Based on these sum rules, we study the importance of vertex corrections to the electron-phonon interaction in a diagrammatic approach. We show that they are crucial for a sum rule for the electron self-energy in the undoped system while a sum rule related to the phonon self-energy of doped systems is satisfied even if vertex corrections are neglected. [1]

[1] O. Rösch *et al.*, Phys. Rev. B (accepted); cond-mat/0607612.

TT 20.65 Wed 14:00 Poster A

One- and two-particle excitations in the doped 2-dim. Hubbard model; a DCA calculation — •Stephan Hochkeppel, Fakher Assaad, and Werner Hanke — University of Wuerzburg, Wuerzburg, Germany

Using the Dynamical Cluster Approximation (DCA) and quantum Monte Carlo as a cluster solver we compute the single particle spectral functions of the electron and hole doped Hubbard model as a function of temperature. We allow U(1) as well as SU(2) symmmetry breaking baths so as to access superconducting states as well as antiferromagnetic order.

Two-particle quantities are computed within an extended RPA scheme where a dynamical vertex is extracted from the cluster and dressed Green function are used to calculate the bubble. The quality of the RPA approach is tested by comparing the resulting Neel temperature to that obtained by allowing for symmetry breaking within the DCA. Furthermore at high temperatures the collective spin excitations are compared with exact Monte Carlo simulations. Finally the temperature dependence of the single particle spectral function from the paramagnetic phase to superconducting state is studied in detail, the aim being a detailed study of the evolution of the pseudogap.

TT 20.66 Wed 14:00 Poster A

Numerical calculation of Wegner estimates for the three-dimensional Bernoulli-Anderson model — •Peter Karmann and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

The Bernoulli-Anderson model is defined as a tight-binding Hamiltonian of non-interacting electrons with a probability distribution of the on-site energies given by a dichotomic or binary measure $\mu = p\delta_0+(1-p)\delta_W$. We study characteristic features of the density of states using various methods for the numerical diagonalization of sparse matrices. In particular, we determine an upper bound of the probability of finding an eigenvalue near a fixed energy for different system sizes and disorder strengths W. Especially for strong disorder, we give a Wegner estimate for resonances which can be identified with finite-size clusters.

TT 20.67 Wed 14:00 Poster A

Pseudogap and the spin-polaron band in the Hubbard model — •Alexei Sherman[1] and Michael Schreiber[2] — [1]Institute of Physics, University of Tartu, 51014 Tartu, Estonia — [2]Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

The spectra of the t-U and t-t'-U Hubbard models are investigated in the one-loop approximation for different values of the electron filling. It is shown that the four-band structure which is inherent in the case of half-filling and low temperatures persists also for some excess or deficiency of electrons. Besides, with some departure from half-filling an additional narrow band of quasiparticle states arises near the Fermi level. The dispersion of the band, its bandwidth and the variation with filling are close to those of the spin-polaron band of the t-J model. For moderate doping spectral intensities in the new band and in one of the inner bands of the four-band structure decrease as the Fermi level is approached which leads to the appearance of a pseudogap in the spectrum.

TT 20.68 Wed 14:00 Poster A

From antiferromagnetism to singlet phase in the Double Bethe lattice — •Hartmut Hafermann[1], Mikhail Katsnelson[2], and Alexander Lichtenstein[1] — [1]I. Institute für Theoretische Physik, Universität Hamburg, D-20355 Hamburg — [2]Institute for Molecules and Materials, Radboud University Nijmegen, 6525 ED Nijmegen, The Netherlands

We consider a model of two coupled Bethe lattices with hopping t on each sublattice, perpendicular hopping $t_\perp$ between the lattices and an on-site repulsion U. We studied the magnetic phase transition from the antiferromagnetic to the non-magnetic state as a function of perpendicular hopping within the Continuous-Time Quantum Monte Carlo approach. For sufficiently large values of U, the transition is found to occur at $t_\perp/t = \sqrt{2}$. By measuring the total spin, it is shown that the non-magnetic state is a singlet state. We further map out the $t_\perp$-U-phase diagram.

TT 20.69 Wed 14:00 Poster A

Wither the sliding Luttinger liquid phase in the planar pyrochlore — •Marcelo Arlego[1] and Wolfram Brenig[2] — [1]Institut für Theoretische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany — [2]Institut für Theoretische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany

Using series expansion based on the flow equation method we study the zero temperature properties of the spin$-1/2$ planar pyrochlore antiferromagnet in the limit of strong diagonal coupling. Starting from the limit of decoupled crossed dimers we analyze the evolution of the ground state energy and the elementary triplet excitations in terms of two coupling constants describing the inter dimer exchange. In the limit of weakly coupled spin$-1/2$ chains we find that the fully frustrated inter chain coupling is critical, forcing a dimer phase which adiabatically connects to the state of isolated dimers. This is inconsistent with a two-dimensional sliding Luttinger liquid phase at finite inter chain coupling.

TT 20.70 Wed 14:00 Poster A

Spinon Deconfinement at the Quantum Critical Point of 2+1 D Antiferromagnets — •Zaira Nazario[1] and David Santiago[2] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Insituut-Lorentz, Leiden University, P.O. Box 9506, NL-2300 RA Leiden, The Netherlands

The natural spin 1 excitations of 2+1 D antiferromagnets are made of constituent confined quarks of spin 1/2, spinons. The quantum paramagnetic phase possesses quantum tunneling events or instantons, which confine the spinons. There have been recent suggestions of new critical points where spinons are deconfined. Instanton events which cause the spinon confinement disappear at the deconfined critical point because the massless spinons screen them effectively and because instanton tunneling becomes infinitely costly. We point out that this happens irrespective of the intrinsic spin of the antiferromagnet. Hence spinons are deconfined irrespective of microscopic spin. Berry phase terms relevant to the paramagnetic phase make the confinement length scale diverge more strongly for half-integer spins, next strongest for odd integer spins, and weakest for even integer spins. There is an emergent photon at the deconfined critical point, but the "semimetallic" nature of critical spinons screens such photon making it irrelevant to long distance physics and the deconfined spinons behave as strictly free particles. A unique prediction critical free spinons at the quantum critical point is an anomalous exponent eta for the susceptibility exactly equal to one.

TT 20.71 Wed 14:00 Poster A

Non-Abelian Statistics in a Quantum Antiferromagnet — •Ronny Thomale and Martin Greiter — Institut für Theorie der Kondensierten Materie, D 76128 Karlsruhe

Non-abelian anyons are traditionally associated with the Pfaffian state for an incompressible quantum Hall state at filling fraction $\nu = 1/2$, a state thought to be realized experimentally in the second Landau level, *i.e.*, at $\nu = 5/2$. The characteristic property is that states with many non-abelian anyons possess an internal degeneracy. The internal space configuration changes as the particles are adiabatically interchanged, *i.e.*, the space is spanned by the different permutations of otherwise identical particles. Since the internal configurations are insensitive to external perturbations which do not move the particles, non-abelian anyons have received exceptional interest in the field of quantum computing. In this work, we present a universality class of two dimensional spin liquids for spin 1 antiferromagnets which support spinon excitations obeying non-abelian statistics. We motivate a Hamiltonian which we expect to stabilize these spin liquids.

TT 20.72 Wed 14:00 Poster A

Auxiliary Fermions and The Popov–Fedotov-Trick: Application to The Phase Diagram of The Bi-Layer Heisenberg Model — •Johannes Reuther, Jan Brinckmann, and Peter Woelfle — Institut f. Theorie der Kondensierten Materie, Universität Karlsruhe

We consider the antiferromagnetic spin-1/2 quantum Heisenberg model for two coupled planes. Each plane consists of spins on a two-dimensional square lattice with a nearest-neighbor coupling $J > 0$, while the planes are connected by another antiferromagnetic coupling $J_\perp$. As is well known, for $J_\perp = 0$ the decoupled planes feature a Néel-like groundstate, while for very large $J_\perp$ the formation of local spin singlets (valence-bond state) is evident.

We use the auxiliary-fermion formulation of spin operators in conjunction with a method proposed by Popov and Fedotov. The latter enables us to take *exactly* into account the auxiliary-particle constraint (i.e., the projection onto the physical Hilbert space).

The ground-state phase diagram of the model is calculated, using a simple diagrammatic approximation for the fermion's self energy. We find a Néel state at small $J_\perp$ and a continuous transition into a valence-bond state (VBS) if $J_\perp$ is increased beyond a critical value. The VBS is characterized by short-range correlations and gapped spin excitations. At the transition point the gap vanishes continuously, and the spin-1 spectrum becomes the magnon dispersion of the Néel state.

The magnetization and the evolution of the spin-excitation spectra as function of $J_\perp$ are compared to the literature.

TT 20.73 Wed 14:00 Poster A

Density functional theory for spinless fermions in one dimension — •Stefan Schenk, Peter Schwab, and Ulrich Eckern — Universität Augsburg

Density functional theory (DFT) within the local density approximation is well known to provide a realistic description of the electronic structure of numerous complex materials, including surfaces and interfaces.

Useful insights into the limitations of DFT can be obtained by considering simple lattice models [1]. In this context, we investigate a one-dimensional model of spinless fermions. An advantage of this model is that the exact exchange-correlation energy of the homogeneous system can be obtained by use of the Bethe-Ansatz. Starting from this exact calculation we employ two methods, the local density approximation and an approximation which includes the exact exchange energy. We compare with results obtained by exact diagonalisation of small systems.

In a next step we include magnetic fields. Therefore we extend the DFT to current density functional theory on a lattice. As in the previous case we investigate the accuracy of our methods by comparison with exact results.

[1] K. Schönhammer, O. Gunnarsson, and R. M. Noack, Phys. Rev. B **52**, 2504 (1995)

TT 20.74 Wed 14:00 Poster A

On Heat Conduction in Spin Chain Compounds — •Peter Jung[1], Rolf Helmes[1], Efrat Shimshoni[2], and Achim Rosch[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Deptartment of Mathematics and Physics, University of Haifa at Oranim, Qiryat-Tivon 36006, Israel

In recent measurements on spin chain compounds an unexpectedly high contribution to the heat conductivity at intermediate temperatures has been observed. Starting point of the presented analysis is the observation that the Spin-1/2 XXZ-model is integrable, resulting in an infinite heat conductivity. Additional couplings destroy the integrability and relax the heat current. We analyze the effect of various couplings on the heat conductivity, with special emphasis on the breakdown of integrability. We aim towards a complete understanding of the mechanisms of relaxation leading to the experimental results, including disorder effects and the coupling to phonons.

TT 20.75 Wed 14:00 Poster A

Spinon confinement and the Haldane gap of SU(n) spin chains — •Stephan Rachel and Martin Greiter — Institut für Theorie der Kondensierten Materie, Universtität Karlsruhe, Postfach 6980, 76128 Karlsruhe, Germany

To begin with, we introduce several exact models for SU(3) spin chains: (1) a translationally invariant parent Hamiltonian involving four-site interactions for the trimer chain, with a three-fold degenerate ground state. We provide numerical evidence that the elementary excitations of this model transform under representation $\bar{\mathbf{3}}$ of SU(3) if the original spins of the model transform under rep. **3**. (2) a family of parent Hamiltonians for valence bond solids of SU(3) chains with spin reps. **6**, **10**, and **8** on each lattice site. We argue that of these three models, only the latter two exhibit spinon confinement and hence a Haldane gap in the excitation spectrum. We generalize some of our models to SU(n). Finally, we use the emerging rules for the construction of VBS states to argue that models of antiferromagnetic chains of SU(n) spins in general possess a Haldane gap if the spins transform under a representation corresponding to a Young tableau consisting of a number of boxes λ which is divisible by n. If λ and n have no common divisor, the spin chain will support deconfined spinons and not exhibit a Haldane gap. If λ and n have a common divisor different from n, it will depend on the specifics of the model including the range of the interaction.

[1] M. Greiter, S. Rachel, and D. Schuricht, submitted to PRB.
[2] M. Greiter and S. Rachel, submitted to PRB.

TT 20.76 Wed 14:00 Poster A

Dominant particle-hole contributions to the phonon dynamics in the spinless one-dimensional Holstein model — •Steffen Sykora, Arnd Hübsch, and Klaus Becker — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

In the spinless Holstein model at half-filling the coupling of electrons to phonons is responsible for a phase transition from a metallic state at small coupling to a Peierls distorted insulated state when the electron-phonon coupling exceeds a critical value. For the adiabatic case of small phonon frequencies, the transition is accompanied by a phonon softening at the Brillouin zone boundary whereas a hardening of the phonon mode occurs in the anti-adiabatic case. The phonon dynamics studied in this poster do not only reveal the expected renormalization of the phonon modes but also show remarkable additional contribu-

tions due to electronic particle-hole excitations.

TT 20.77 Wed 14:00 Poster A

The one-dimensional Hubbard model: A benchmark for variational cluster approximations — •Matthias Balzer, Michael Potthoff, and Werner Hanke — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland D-97074 Würzburg

Important physical properties of lattice models of strongly correlated electrons are often dominated by short-range spatial correlations. Starting from the purely local (atomic) physics, short-range correlations can be included step by step within cluster approximations generated by the self-energy-functional theory. The one-dimensional Hubbard model is considered to benchmark various cluster schemes: the plain cluster perturbation theory (CPT), the variational cluster approach (VCA) using different sets of variational parameters as well as extensions of the VCA including bath degrees of freedom. Calculations are performed at zero temperature for clusters up to 10 sites. The results for the filling dependence of the chemical potential and the transition to the Mott insulator are compared to the exact Bethe ansatz. Several questions concerning thermodynamical consistency, cluster boundary conditions, optimal choice of variational parameters, spectral functions etc. are investigated. The applications of variational cluster methods for the study of the filling-controlled Mott transition in two dimensions are discussed.

TT 20.78 Wed 14:00 Poster A

Efficient simulation of one-dimensional many-body quantum systems — •Alex Cojuhovschi, Malcolm Einhellinger, and Eric Jeckelmann — Institut für Theoretische Physik, Leibniz Universität Hannover

Vidal's time-evolving block decimation (TEBD) algorithm allows for the accurate simulation of the ground state and the time evolution in one-dimensional many-body quantum systems. Although density-matrix renormalization group (DMRG) methods seem more versatile and efficient than the TEBD algorithm on sequential computers, extensively parallelized DMRG codes have shown a good scalability only up to 8 or 16 processors, which severely restricts their use on modern parallel supercomputers. We show that the TEBD algorithm can be easily parallelized and has a much better scalability than DMRG codes for large systems. This could enable the use of massively parallel computers for this type of simulations.

Furthermore, we have investigated the time-evolution of the density-matrix spectrum in non-interacting electron systems out of equilibrium such as two reservoirs coupled through a quantum dot. This allows us to devise more efficient procedures for simulating large non-interacting subsystems (such as charge or heat reservoirs) in DMRG and TEBD approaches to the time evolution of quantum systems.

TT 20.79 Wed 14:00 Poster A

Deconvolution procedures for dynamical DMRG spectra — •Martin Paech and Eric Jeckelmann — Institut fuer Theoretische Physik, Leibniz Universitaet Hannover

The dynamical density-matrix renormalization group (DDMRG) method provides the frequency-dependent correlation functions of finite-size low-dimensional systems with great accuracy. The spectrum of an infinite system can be obtained for each frequency separately using a finite-size scaling analysis of the DDMRG data. We have shown previously that the infinite-system spectrum can sometimes be obtained at a much lower computational cost by a deconvolution of the finite-system DDMRG data under some regularity assumptions for the spectrum. Although standard algorithms for inverse problems such as a deconvolution yield good results for smooth continuous spectra they fail if the spectrum includes singularities. We discuss several deconvolution procedures for general spectra and illustrate them with a study of the density of states in one-dimensional correlated electron systems.

TT 20.80 Wed 14:00 Poster A

Improved scaling for the Matrix Product State alternative to DMRG — •Peter Pippan[1], Steven White[2], and Hans Gerd Evertz[1] — [1]Theor. and Comput. Physics, TU Graz, 8010 Graz, Austria — [2]Dept of Physics and Astronomy, UC Irvine, CA 92697, USA

The density-matrix renormalization group (DMRG) is a highly efficient algorithm for the investigation of low-dimensional, strongly correlated systems. It converges to the ground state, which can be written as a matrix product state. We study a recently proposed variational method that optimizes these matrix product states independently of DMRG. This method proofs useful for periodic boundary conditions and is conceptually more powerfull than DMRG, but is numerically much less efficient. We introduce a decomposition of large matrices using a singular value decomposition (SVD). Neglecting small singular values, we approximate the matrices very accurately while keeping storage requirements small. The computational effort and especially its scaling with system size is then drastically reduced, while accuracy remains unchanged. This allows the investigation of much larger systems with periodic boundary conditions. Properties of the new method are studied for the Spin 1 Heisenberg chain.

TT 20.81 Wed 14:00 Poster A

Phonon simulations with arbitrary dispersions — •Hans Gerd Evertz, Franz Michel, and Peter Pippan — Theoretical and Computational Physics, TU Graz, 8010 Graz, Austria

We describe a new Quantum Monte Carlo method that allows the efficient simulation of phonons with arbitrary bare dispersion, coupled to spins in any dimension, or to 1d electrons.

We examine the spin Peierls transition in 1d in the case of optical phonons and of acoustical phonons and show that it occurs at the *same* coupling. Detailed phonon spectra exhibit both a central peak and softening, depending on the bare phonon frequency at momentum π. In 2d we examine the stripe pattern of coupled chains. We contrast the behavior of spin-phonon systems to that of coupled electrons and phonons.

TT 20.82 Wed 14:00 Poster A

Fermi-edge singularities in the mesoscopic regime — •Martina Hentschel — MPIPKS Dresden, Nöthnitzer Str. 38, 01187 Dresden

Motivated by the experimental progress in the field of mesoscopic physics and quantum chaos over the past years, we study the many-body effects contributing to Fermi-edge singularities in the x-ray edge problem for mesoscopic systems and compare the results with the well-understood metallic case. Upon absorption of an x-ray, a core electron is excited into the conduction band, and the core hole left behind constitutes a sudden, localized perturbation. It entails two counteracting many-body responses, namely Anderson orthogonality catastrophe and Mahan's exciton, that affect the photoabsorption cross section. Using a rank-one model and a Fermi golden rule approach, we find characteristic deviations from the metallic case that originate in the small system size, mesoscopic fluctuations, and most notably the coherent dynamics of conduction electrons in mesoscopic systems like quantum dots or metallic nanoparticles. We investigate the dependence of the photoabsorption spectra on the number of electrons and argue that our predicitons are observable using nowadays experimental technology.

TT 20.83 Wed 14:00 Poster A

Anderson Orthogonality Catastrophe in Mesoscopic Systems — •Georg Röder, Swarnali Bandopadhyay, and Martina Hentschel — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany

Anderson orthogonality catastrophe (AOC) is an universal many-body response of an electron gas subject to a sudden, localised perturbation. It refers to the vanishing of overlap of the unperturbed and perturbed many-body ground states in the thermodynamic limit. Here, we study AOC in mesoscopic systems where the finite number of electrons, the confining geometry, interference effects and mesoscopic fluctuations give rise to novel behaviours not seen in bulk systems. In particular we consider two dimensional regular structures such as disc-like and rectangular quantum wells and realistic few electron quantum dots with parabolic confinement potential. Comparing the results with the chaotic case [M. Hentschel, D. Ullmo, and H. U. Baranger, Phys. Rev. Lett. **93**, 176807 (2004)], we find characteristic differences such as shell effects. Our model of a rank-one perturbation describes, e.g., the core hole created in a x-ray absorption process where the AOC response of the system is experimentally accessible through the photoemission cross section.

TT 20.84 Wed 14:00 Poster A

Low-density expansion for the two-dimensional electron gas — •Francesca Sauli and Peter Kopietz — Institut für Theoretische Physik, J.W. Goethe Universität, Frankfurt am Main

We show that in two dimensions ($2D$) a systematic expansion of the self-energy and the effective interaction of a dilute electron gas in pow-

ers of the two-body T-Matrix T_0 can be generated from an exact hierarchy of the functional renormalization group equations for one-particle irreducible vertices using the chemical potential as flow parameter. Due to the interference of particle-particle and particle-hole channels at order $T_0 2$, in $2D$ the ladder approximation for the self-energy is not reliable beyond the leading order in T_0. We also discuss two-body scattering in vacuum in arbitrary dimensions from the renormalization group point of view and argue that the singular interaction proposed by Anderson [Phys. Rev. Lett. **65**, 2306 (1990)] cannot be ruled out on the basis of the ladder approximation.