TT 6: Postersession Correlated Electrons: (General) Theory, Low-Dimensional Systems, Kondo Physics, Heavy Fermions, Quantum-Critical Phenomena

Time: Monday 13:00–16:45 Location: P1A

TT 6.1 Mon 13:00 P1A

Magnetic and electronic properties of double perovskites $La_{2-x}Sr_xCoIrO_6 (0 \leq x \leq 1)$ — •Narendirakumar Narayanan[1,2], Robert Laskowski[3], Daria Mikhailova[1,2], Anatoly Senyshin[1], Peter Blaha[3], Karlheinz Schwarz[3], Helmut Ehrenberg[1,2], and Hartmut Fuess[1] — [1]Darmstadt University of Technology, Department of Materials Science — [2]IFW Dresden, Institute for Complex Materials — [3]Vienna University of Technology, Institute of Materials Chemistry

Double Perovskites (DP) $A_2BB'O_6$ with 3d transition metals at B-site and 4d or 5d transition metals at B'-site have been extensively studied due to their interesting physical properties, that could be tuned by the partial substitution of the ions involved[1-2]. The ability of Iridium to display different oxidation states and structural constraints (distortion of bond angles) on 5d orbitals, which are generally considered more extended in nature compared to the 3d or 4d ones promise interesting physical properties. We discuss the composition La_2CoIrO_6 in terms of density functional theory (DFT). We focus mainly on two open aspects. The first one concerns the realization of an insulating state in this material. We show that insulating state can develop only, if we apply LDA/GGA+U method for both B and B' atoms. The second aspect concerns the magnetic properties. Calculations indicate that this DP has a non-collinear magnetic structure.

[1] K.-I. Kobayashi, T. Kimura, H. Sawada, K. Terakura and Y. Tokura, Nature 395, 677 (1998).

[2] H. Kato, T. Okuda, Y. Okimoto, Y. Tomioka, K. Oikawa, T. Kamiyama, and Y. Tokura, Phys. Rev. B 65, 144404 (2002).

TT 6.2 Mon 13:00 P1A

Novel unitary transformations to treat systems with quasiparticles of finite lifetime — Tim Fischer[1], •Nils Drescher[1], Sebastian Duffe[1], and Götz S. Uhrig[1,2] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, 44221 Dortmund, Germany — [2]School of Physics, University of New South Wales, Kensington 2052, Sydney NSW, Australia

The method of self-similar continuous unitary transformations maps a given Hamiltonian to an effective Hamiltonian whose final structure depends on the generator of the unitary transformation. The aim is to derive an effective Hamiltonian simpler than the original Hamiltonian without losing its physics. One route is to disentangle sectors of different number of quasiparticles which is achieved by the MKU generator [1,2]. But this route fails if the elementary excitations have a finite lifetime due to hybridization with continua which is a common situation in physics.

We propose variants of the MKU generator and prove that they lead to converging flow equations. The new unitary transformations are tested and illustrated for one-dimensional spin models.

[1] A. Mielke, Eur. Phys. J. B 5, 605 (1998)

[2] C. Knetter, G.S. Uhrig, Eur. Phys. J. B 13, 209 (2000)

TT 6.3 Mon 13:00 P1A

Nonequilibrium steady-state density of states of the Falicov-Kimball model in the presence of a large electric field — •Alexander Joura[1] and Jim Freericks[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Georgetown University, Washington, DC 20057, U.S.A.

The electronic density of states (DOS) of the Falicov-Kimball model in a constant uniform electric field E is calculated using a Kadanoff-Baym-Keldysh nonequilibrium Green's function technique and dynamical mean-field theory. When the electron-electron interaction U vanishes, the DOS is the Wannier-Stark ladder of delta functions spaced by the Bloch frequency. If U is increased, the delta function peaks initially broaden due to the scattering, but ultimately evolve into a continuous structure for large U's. As E is increased from small values, where linear response theory can be used and we see broadened Wannier-Stark peaks, the DOS develops a shape with large peaks at miniband edges, separated in energy by U. We verify the accuracy of our calculations by checking the DOS against frequency-moment sum rules, and an independent transient-response calculation of the Green's functions at long times. While our formalism has been applied to the Falicov-Kimball model, it can also be directly extended to other models like the Hubbard or periodic Anderson model, by using more complicated impurity problem solvers.

TT 6.4 Mon 13:00 P1A

Charge transport in classical geometrically frustrated systems — •David Leipold and Erich Runge — TU-Ilmenau, Institut für Physik, D-98693 Ilmenau

The quantum mechanics of geometrically frustrated systems has been studied intensively in recent years [1,2]. Here, we study classical charge transport on the criss-crossed checkerboard lattice, which is the two-dimensional counterpart of the pyrochlore lattice. We present results obtained by Monte Carlo simulations in a wide range of particle densities, applied voltages and temperatures. Furthermore, we discuss analytical models which reproduce the simulated behavior in various limits. Our simulations confirm the existence of a number of structures, which are classical analogues of quantum mechanical quasi-particles. These were predicted earlier [3] to carry fractional charge. Due to their high mobility, they contribute substantially to charge transport.

[1] E. Runge and P. Fulde, Phys. Rev. B **70**, 245113 (2004)

[2] F. Pollmann, P. Fulde, E. Runge, Phys. Rev. B **73**, 125121 (2006)

[3] F. Pollmann, J.J. Betouras, E. Runge, Phys. Rev. B **73**, 174417 (2006)

TT 6.5 Mon 13:00 P1A

Matrix product state calculation of the correlation density matrix: an unbiased analysis of long-range correlations — •Wolfgang Münder[1], Andreas Weichselbaum[1], Jan von Delft[1], and Christopher Henley[2] — [1]Department of Physics and Center for NanoScience, Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilans-Universität, Theresienstrasse 37, 80333 Munich — [2]LASSP, Clark Hall, Cornell University, Ithaca, NY 14853-2501

A useful concept for determining the dominant correlations of the ground state wave function of a lattice model, in an unbiased fashion without prior knowledge, is the correlation density matrix (CDM) [1]. For two disjoint, separated clusters A and B, it is defined to be the density matrix of their union, minus the direct product of their respective density matrices, $\rho_{AB}^{CDM} = \rho_{A\cup B} - \rho_A \otimes \rho_B$. It encodes all possible correlations between the clusters A and B and has block-diagonal form, dictated by the symmetries of the Hamiltonian. We analyse it for a family of interacting spinless fermion models on a ladder [1], which has nontrivial mappings to free fermions in certain limits [2]. We use the density matrix renormalization group (implementing Abelian symmetries explicitly) to calculate the ground state in the form of a matrix product state, from which the correlation density matrix can straightforwardly be obtained. We also discuss methods for extracting the Luttinger liquid scaling exponents from the correlation density matrix.

[1] S.-A. Cheong and C.L. Henley, arXiv:0809.0075v1 (2008).

[2] S.-A. Cheong, PhD thesis, Cornell Univ., (2007), http://people.ccmr.cornell.edu/~clh/Theses/cheong-habis.pdf

TT 6.6 Mon 13:00 P1A

A fast impurity solver based on merging the equation of motion method and genetic algorithms — •Qingguo Feng, Yuzhong Zhang, and Harald O. Jeschke — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

The successful application of LDA+DMFT to strongly correlated systems generates increasing interest in the development of fast impurity solvers for DMFT. By using the equation of motion method with a suitable decoupling scheme, a new fast impurity solver is established. An efficient way to find self-consistent solutions of the closed set of integral equations is found in a combination of iteration and genetic algorithms. This new impurity solver can work directly on the real frequency axis and yields the Green's function for all temperatures. The successful description of various physical properties of Hubbard and periodic Anderson models demonstrates the power of our method in understanding strongly correlated systems.

TT 6.7 Mon 13:00 P1A

CDMFT and DCA with Lanczos solver — •Giorgio Sangiovanni[1], Erik Koch[2], and Olle Gunnarsson[3] — [1]Vienna University of Technology — [2]Forschungszentrum Jülich — [3]Max-Planck Institut Stuttgart

Quantum cluster methods are among the most powerful tools to study strongly correlated systems. While a huge variety of impurity-solver are available nowadays for single-site Dynamical Mean Field Theory, for Cellular Dynamical Mean Field Theory (CDMFT) and Dynamical Cluster Approximation (DCA) only Quantum Monte Carlo-based solvers are usually employed. Exact Diagonalization has been hitherto used only for extremely small clusters. We introduce Hamiltonian-based solver using Lanczos at T=0 exploiting the cluster point symmetry. This implies symmetries of the hybridization, which can substantially reduce the number of independent parameters to fit the bath Green function. We review these symmetries and derive general sum-rules for the hybridizations, which (i) allow to check the quality of a fit using a finite set of bath sites and (ii) imply what hybridizations vanish. Such rationalization of the Lanczos solver is a necessary step towards a more efficient algorithm which may eventually allow us to treat larger systems.

TT 6.8 Mon 13:00 P1A

Superconductivity in the two-dimensional extended periodic Anderson model — •Nham Phan Van[1,2] and Klaus W Becker[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Max-Planck Institut für Physik komplexer Systeme, D-01187 Dresden, Germany

The two-dimensional periodic Anderson model with an additional local Coulomb repulsion U_{fc} between localized f and conduction electrons is investigated by the use of the projector-based renormalization method. When the f-level energy ϵ_f is close to the Fermi level, the valence transition becomes sharper by increasing U_{fc}. We start from an Hamiltonian which includes small gauge symmetry breaking fields and derive self-consistent equations for the order parameters. Our numerical results show that the d-wave superconducting order is dominant close to the sharp valence transition regime. This affirms that the valence fluctuations might lead to superconductivity in the Ce based heavy-fermion systems under high pressure.

TT 6.9 Mon 13:00 P1A

Thermodynamics and transport properties of the single-band Hubbard model — •Ken Lichtner and Wolfgang Nolting — Institut für Physik, Humboldt-Universität, Newtonstraße 15, 12489 Berlin, Germany

We study the possibility and stability of band-ferromagnetism in the single-band Hubbard model, focusing on thermodynamics as well as transport properties calculated fully self-consistently within our "local modified perturbation theory". The obtained self energy fulfills the first four spectral moments, therewith guaranteeing the correct high-energy behaviour, and is exact up to second order perturbation theory. Results are presented for f.c.c. as well as s.c. lattices. Phase diagrams are shown for ferromagnetic and paramagnetic solutions presented in terms of finite T and n. An overall comparison with the dynamical mean-field theory for infinite-dimensional lattices (DMFT) and the simple mean field theory (Stoner) is drawn.

TT 6.10 Mon 13:00 P1A

Slyanin isomorphism and a correspondence between coordinate and functional Bethe ansatz — •Andreas Osterloh — Institut für theoretische Physik, Leibniz Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany.

We focus on the Sklyanin functional Bethe ansatz (FBA) from a different point of view, interpreting it as a coordinate Bethe ansatz (CBA) tailored from algebraic insight. This perspective sheds light on the Sklyanin isomorphism and establishes a direct access to the eigenstates. The isomorphism unveils the meaning of the Sklyanin Q-functions and shows that the resulting T-Q recursion relations can be extended at the best convenience to outside the Sklyanin FBA lattice.

TT 6.11 Mon 13:00 P1A

Antiferroquadrupolar phases in $U(Pd_{1-x}Pt_x)_3$, $x \leq 0.01$ — •Markus Schäpers[1], Matthias Bleckmann[1], Dirk Schulze Grachtrup[1], Stefan Süllow[1], and Keith McEwen[2] — [1]Technsiche Universität Braunschweig, Braunschweig, Deutschland — [2]University College London, London, England

The double hexagonal compound UPd_3 has been shown to undergo several successive phase transitions below 8 K. These low temperature phases are antiferroquadrupolar ordered ones with different AFQ order parameters. In-field measurements on UPd_3 reveal a complex response of these phases on magnetic fields, leading to a very rich magnetic phase diagram [1-3].

Here, for the first time we present resistivity measurements and a magnetic phase diagram for single crystalline lowly doped samples $U(Pd_{1-x}Pt_x)_3$, $x \leq 0.01$, and compare these measurements to pure UPd_3. We find that doping leads to reduced ordering temperatures but leaves the underlying physics of the AFQ ordered phases unaffected

[1] Y. Tokiwa, K. Sugiyama, T. Takeuchi, M. Nakashima, R. Settai, Y. Inada, Y. Haga, E. Yamamoto, K. Kindo, H. Harima and Y. Onuki, J. Phys. Soc. Jpn. 70 (2001) 1731

[2] D. F. McMorrow, K. A. McEwen, U. Steigenberger, H. M. Rønnow and F. Yakhou, Phys. Rev. Lett. 87 (2001) 057201

[3] H. C. Walker, K. A. McEwen, D. F. McMorrow, S. B. Wilkins, F. Wastin, E. Colineau and D. Fort, Phys. Rev. Lett. 97 (2006) 137203

TT 6.12 Mon 13:00 P1A

Structural relaxation due to electronic correlations in the paramagnetic insulator $KCuF_3$ — •Ivan Leonov[1], Nadia Binggeli[2,3], Dmitry Korotin[4], Vladimir I. Anisimov[4], Natasa Stojic[5,3], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany — [2]Abdus Salam International Center for Theoretical Physics, 34014 Trieste, Italy — [3]INFM-CNR Democritos, 34014 Trieste, Italy — [4]Institute of Metal Physics, 620219 Yekaterinburg GSP-170, Russia — [5]International School for Advanced Studies, SISSA, 34014 Trieste, Italy

We present a computational scheme for the investigation of complex materials with strongly interacting electrons which is able to treat atomic displacements, and hence structural relaxation, caused by electronic correlations [1]. It combines *ab initio* band structure and dynamical mean-field theory and is implemented in terms of plane-wave pseudopotentials. Results obtained for paramagnetic $KCuF_3$, namely an equilibrium Jahn-Teller distortion of 4.2% and antiferro-orbital ordering, agree well with experiment. The electronic correlations are also found to be responsible for a considerable enhancement of the orbital polarization. The GGA+DMFT scheme presented here opens the way for fully microscopic investigations of the structural properties of strongly correlated electron materials such as lattice instabilities observed at correlation induced metal-insulator transitions.

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

TT 6.13 Mon 13:00 P1A

Phonon renormalization from local and transitive electron-lattice couplings in strongly correlated systems — •Ernst von Oelsen[1], Andrea Di Ciolo[2,3], Jose Lorenzana[2,3,4], Marco Grilli[2,3], and Götz Seibold[1] — [1]Institut für Physik, BTU Cottbus, PBox 101344, 03013 Cottbus, Germany — [2]Dipartimento di Fisica, Università di Roma "La Sapienza", P. Aldo Moro 2, 00185 Roma, Italy — [3]SMC-Istituto Nazionale di Fisica della Materia — [4]ISC-Consiglio Nazionale delle Ricerche

Within the time-dependent Gutzwiller approximation (TDGA) applied to Holstein- and SSH-Hubbard models we study the influence of electron correlations on the phonon self-energy. For the local Holstein coupling we find that the phonon frequency renormalization gets weakened upon increasing the onsite interaction U for all momenta. In contrast, correlations can enhance the phonon frequency shift for small wave-vectors in the SSH-Hubbard model. Moreover the TDGA applied to the latter model provides a mechanism which leads to phonon frequency corrections at intermediate momenta due to the coupling with double occupancy fluctuations. Both models display a shift of the nesting-induced to a $q = 0$ instability when the onsite interaction becomes sufficiently strong and thus establishing phase separation as a generic phenomenon of strongly correlated electron-phonon coupled systems.

TT 6.14 Mon 13:00 P1A

Calculation of thermoelectric properties by LDA+DMFT — •Philipp Wissgott, Philipp Hansmann, Nico Parragh, Alessandro Toschi, and Karsten Held — Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria

Strongly correlated electron systems were recently found to show im-

pressive thermoelectric properties. For example the transition metal oxides Na_xCoO_2 [1] and $LiRh_2O_4$ [2] have a thermopower of almost 100 μV/K. As bandstructure and electronic correlations can play an important role for the thermopower, we investigate these materials with the combination of density functional theory and dynamical mean field theory. Following [3], effects of Na disorder, which lead to stronger correlations, are taken into account by a binary distribution. In comparison to experiment, we present results for the thermopower, the resistivity, and the thermal conductivity at various temperatures.

[1] I. Terasaki, Y. Sasago and K. Uchinokura, Phys. Rev. B **56**, R12685 (1997).

[2] Y. Okamoto *et al.*,Phys. Rev. Lett. **101** 086404 (2008).

[3] C.A. Marianetti and G. Kotliar, Phys. Rev. Lett. **98** 176405 (2007).

TT 6.15 Mon 13:00 P1A

Electronic structure of the low-dimensional transition metal oxyhalide VOCl — •Sebastian Glawion[1], Markus Scholz[1], Karin Goss[1], Michael Sing[1], Harald Jeschke[2], Tanusri Saha-Dasgupta[3], Roser Valenti[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg — [2]Institut für Theoretische Physik, Universität Frankfurt — [3]S.N. Bose National Centre for Basic Sciences, Kolkata, India

In the quest for RVB-like superconductivity, layered oxyhalides of the form MOX (M=Ti,V; X=Cl,Br) have been discussed some fifteen years ago as possible candidates. This was due to their low-dimensional crystal structure involving frustrated triangular lattice planes. While no superconducting state in these Mott insulators was observed yet, other interesting phenomena, e.g. an unconventional spin-Peierls transition, have been found in TiOX. The isostructural material VOCl has a $3d^2$ configuration and shows antiferromagnetic ordering below 150K; magnetic susceptibility measurements show an anisotropy along the a-axis. Electronically, however, the degree of one-dimensionality observed by photoemission is reduced compared to the well-studied $3d^1$ TiOX systems. LDA+U calculations indicate that VOCl is a Mott insulator despite its two 3*d* electrons. Upon n-doping with alkali metals new states appear in the gap without having quasi-particle character, i.e. no evidence for a metallic phase is found. A comparison between VOCl and TiOX is expected to yield new insights into the importance of one-dimensionality and multi-band Mott-Hubbard physics in the oxyhalides.

TT 6.16 Mon 13:00 P1A

Electronic properties of Fe, Mn, and Ni impurities in MgO thin films — T. Haupricht[1], •Y.-Y. Chin[1,2], R. Gierth[1], J. Weinen[1], S. G. Altendorf[1], A. Hendricks[1], Z. Hu[1], J. Gegner[1], H. Fujiwara[1], D. Regesch[1], H. H. Hsieh[3], H.-J. Lin[2], C. T. Chen[2], and L. H. Tjeng[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]Chung Cheng Institute of Technology, National Defense University, Taoyuan, Taiwan

Transition metal ions in MgO can serve as model systems for various (usually more complicated) d^n systems in octahedral symmetry. Going from bulk crystals to impurity systems the core level and valence band photoemission (PES) and soft x-ray absorption (XAS) spectra can change significantly e.g. due to the absence of non-local screening effects [v. Veenendaal et al., PRL 70 (1993)]. Here, we present our core level and valence band PES and XAS data of Fe, Mn, and Ni impurities in MgO thin films grown on metal substrates in-situ by means of molecular beam epitaxy (MBE). Compared to the bulk compounds FeO, MnO, and NiO, remarkable differences are observed in the spectra. In order to understand these differences we have simulated the spectra using configuration interaction cluster calculations. Ab-initio oriented approaches such as LDA+DMFT are highly desired to obtain parameter free explanations.

TT 6.17 Mon 13:00 P1A

Ultrasonic investigation of the quasi-2D quantum antiferromagnet Cs_2CuCl_4 — •A. Sytcheva[1], S. Zherlitsyn[1], J. Wosnitza[1], O. Chiatti[1], A. A. Zvyagin[2,3], and R. Coldea[4] — [1]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, Germany — [2]MPI für Physik komplexer Systeme, Dresden, Germany — [3]Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine — [4]Wills Physics Laboratory, University of Bristol, United Kingdom

We report on results of sound-velocity and sound-attenuation measurements in the triangular-lattice quasi-2D spin-1/2 antiferromagnet (AFM) Cs_2CuCl_4 ($T_N = 0.6$ K), in magnetic fields up to 18 T applied along the *a* axis and at low temperatures from 5 down to 0.3 K. Below T_N this material displays a 3D incommensurate spiral long-range AFM order, which is stable up to $B_s \approx 8.5$ T for fields applied along the *a* axis. Above this field all spins are polarized. For the AFM phase a possibility for the Bose-Einstein condensation of magnons has been suggested whereas beyond the AFM phase at low temperatures a proximity to the spin liquid (SL) state is considered in this compound. The longitudinal c_{11} acoustic mode, which has a propagation direction along the *a* axis, shows pronounced anomalies in sound velocity and attenuation in discussed temperature and field range indicating spin-strain interaction. It also demonstrates frequency-dependent effects indicating the presence of relaxation processes. The ultrasonic results are analyzed with a theory based on exchange-striction coupling. There is a good qualitative agreement between theory and experiment.

TT 6.18 Mon 13:00 P1A

Effects of structural modulations on the quasiparticle distribution in 2H-$TaSe_2$ — •Torben Hänke[1], Alexander Kordyuk[1], Volodymyr Zabolotnyy[1], Daniil Evtushinsky[1], Paul Sass[1], Christian Hess[1], Sergey Borisenko[1], Helmut Berger[2], and Bernd Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany — [2]Institut de Physique Appliquée, EPF, 1015 Lausanne, Switzerland

We report on a temperature dependent scanning tunneling microscopy (STM) and angle resolved photoemission (ARPES) study of the Cu intercalated dichalcogenide 2H-$TaSe_2$. The Cu intercalation leads not only to a lowering of the transition temperature into the commensurate charge-density wave state (CDW) but also to the formation of a $\sqrt{13} \times \sqrt{13}$ superstructure, previously observed for the 1T polytype only [1]. The origin, spectroscopic appearance, and influence of these superstructures on the electronic properties of 2H-$TaSe_2$ will be discussed.

[1] D. Stoltz *et al.*, Phys. Rev. B **76** 073410 (2007).

TT 6.19 Mon 13:00 P1A

Low temperature magnetism of $La_{1-x}Sr_xCoO_3$ ($x \sim 0.002$) — •V. Kataev[1], A. Alfonsov[1], E. Vavilova[1,2], B. Büchner[1], A. Podlesnyak[3], M. Russina[3], A. Furrer[4], Th. Strässle[4], E. Pomjakushina[4,5], K. Conder[5], and D.I. Khomskii[6] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical Technical Institute, RAS, 420029 Kazan, Russia — [3]Hahn–Meitner–Institut, D-14109 Berlin, Germany — [4]Laboratory for Neutron Scattering, ETH Zürich & PSI, CH-5232 Villigen PSI, Switzerland — [5]Laboratory for Developments and Methods, PSI, CH-5232 Villigen PSI, Switzerland — [6]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

We present results of electron spin- (ESR), nuclear magnetic resonance (NMR) and inelastic neutron scattering (INS) studies of single crystals of $La_{1-x}Sr_xCoO_3$. In contrast to $LaCoO_3$, which is nonmagnetic at $T \lesssim 30$ K, a very small Sr^{2+} doping ($x \sim 0.002$) yields a strong magnetization already at low T. ^{59}Co NMR measurements indicate the formation of extended magnetic clusters in this temperature regime. ESR spectroscopy reveals multiple gapped resonance excitations with different g-factor values suggesting that magnetic clusters have a large spin multiplicity and substantial spin-orbital coupling. The Q-dependence of the INS intensity gives evidence that the cluster comprises 7 magnetic Co ions. We argue that the doped hole couples these ions ferromagnetically yielding a spin-state polaron with a huge local magnetic moment.

TT 6.20 Mon 13:00 P1A

Collective two-particle excitations in cuprates and manganites: Resonant inelastic x-ray scattering and electron energy loss spectroscopy — •Jochen Geck[1], Roberto Krauss[1], Roman Schuster[1], Martin Knupfer[1], Patrick Ribeiro[1], Bernd Büchner[1], Pieter Glatzel[2], Javier Herrero-Martin[2], Joaquin Garcia-Ruiz[3], Diego Casa[4], Thomas Gog[4], Hiroki Wadati[5], and George A. Sawatzky[5] — [1]IFW Dresden, Germany — [2]European Synchrotron Radiation Facility, France — [3]Universidad de Zaragoza, Spain — [4]Advanced Photon Source, USA — [5]University of British Columbia, Canada

The two-particle charge excitations of Sr_2CuO_3, which contains one-dimensional corner-sharing CuO_2-chains, were studied by Resonant Inelastic X-ray Scattering (RIXS) at the Cu K-edge. At the center of the Brillouin zone, the dependence of the various charge-transfer excitations on the incident photon energy E_i was studied in detail. The

different charge transfer excitations resonate for different intermediate states, i.e., different E_i, which allows to draw conclusions about the symmetry of the created excitations. Further, the RIXS results are discussed in comparison to previous Electron Energy Loss Spectroscopy (EELS) studies. A similar approach was then used to investigate the two-particle excitations $(La,Sr)_2MnO_4$. Surprisingly, the excitations observed for the doped manganite materials share similar traits with the ones observed for the doped cuprates.

TT 6.21 Mon 13:00 P1A

Specific heat of a Cu_3 spin tube — •Juergen Schnack[1] and Roman Schnalle[2] — [1]Universität Bielefeld, Fakultät für Physik, Postfach 100131, D-33501 Bielefeld — [2]Universität Osnabrück, Fachbereich Physik, D-49069 Osnabrück

$[(CuCl_2tachH)_3Cl]Cl_2$ is a frustrated three-leg spin tube of antiferromagnetically coupled Cu spins with $s = 1/2$ [1,2]. The $T = 0$ phase diagram (gaps, plateaus) was discussed in e.g. [3,4]. Here we report on the specific heat of the spin tube which was determined experimentally. For low temperatures the specific heat is linear in temperature – reminiscent of a one-dimensional gapless spin chain – followed by a pronounced peak at higher temperatures. This behavior is discussed theoretically.

[1] J. Schnack *et al.*, Phys. Rev. B **70**, 174420 (2004).
[2] J. Schnack, C. R. Chimie **10**, 15 (2007).
[3] A. Lüscher *et al.*, Phys. Rev. B **70**, 060405(R) (2004).
[4] J.-B. Fouet *et al.*, Phys. Rev. B **73**, 014409 (2006).

TT 6.22 Mon 13:00 P1A

High Magnetic Field Measurements on single crystalline (5-MAP)$_2$CuBr$_4$ — •Daniela Rauch[1], Jan Kreitlow[1], Yurii Skourski[2], Mark M. Turnbull[3], and Stefan Süllow[1] — [1]Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, Braunschweig — [2]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, Dresden — [3]Carlson School of Chemistry and Biochemistry, Clark University, Worcester, USA

(2-amino-5-methylpyridinium)$_2$CuBr$_4$, abbreviated as (5-MAP)$_2$CuBr$_4$, has been characterized as a square S=1/2 Heisenberg antiferromagnetic lattice [1,2]. The compound consists of two-dimensional sheets of highly distorted $CuBr_4$ tetrahedra separated by the organic cations. The magnetic coupling constants are 6.5 K for the intra-sheet coupling, 1.5 K for a residual inter-sheet coupling, with both interactions in effect resulting in an antiferromagnetic transition occurring at T_N=3.8 K.

Here we report a single crystal high magnetic field study on (5-MAP)$_2$CuBr$_4$, with magnetic fields up to 40 T at temperatures down to 1.5 K. From the data additional information on local anisotropies such as of the g-factor can be obtained and will be discussed.

[1] H. Place, R. Willett, Acta Cryst. **C43** (1987) 1050.
[2] F.M. Woodward, A.S. Albrecht, C.M. Wynn, C.P. Landee, M.M. Turnbull, Phys. Rev. B **65** (2002) 144412

TT 6.23 Mon 13:00 P1A

Specific heat of the highly anisotropic antiferromagnet [Cu(pyz)$_2$(HF$_2$)]PF$_6$ — •R. Beyer[1], M. Uhlarz[1], J. Wosnitza[1], and J.A. Schlueter[2] — [1]Hochfeld-Magnetlabor (HLD), Forschungszentrum Dresden-Rossendorf (FZD), Dresden, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, USA

The metal-organic compound $[Cu(pyz)_2(HF_2)]X$ with $X = PF_6$ exhibits a quasi-cubic lattice of copper ions ($S = \frac{1}{2}$), but the magnetic properties show a predominantly two-dimensional (2D) nature due to a large anisotropy in the exchange couplings. The magnetic entropy and the antiferromagnetic ordering, eventually occurring at about 4.4 K, were investigated by specific-heat measurements. For this we established a continuous relaxation-time technique, using a single relaxation process to get specific heat data over a wide temperature range. The calorimetric investigations, performed between 2 and 100 K and in magnetic fields up to 14 T, have revealed a non-monotonic field dependence of the ordering temperature. The results are as expected from the model for a $S = \frac{1}{2}$ 2D square-lattice quantum Heisenberg antiferromagnet with an additional weak interlayer exchange (via Cu-F-H-F-Cu bonds).

In comparison to the $X = BF_4$ compound, the antiferromagnetically ordered phase extends to much higher temperatures. In a more detailed analysis, we can extract all exchange interactions with an interlayer coupling ten times larger than in $X = BF_4$. Thus, the 2D character is significantly reduced in $X = PF_6$.

TT 6.24 Mon 13:00 P1A

From solid to cluster – a computational study on the model compound Li_2CuO_2 — •Ulrike Nitzsche[1], Stefan-Ludwig Drechsler[1], and Helge Rosner[2] — [1]IFW Dresden, PF 270116, 01171 Dresden — [2]MPI CPfS Dresden, Nöthnitzer Str. 40, 01187 Dresden

The treatment of strong electron correlations is one of the major challenges in modern solid state physics and chemistry. Two standard approaches tackle the problem from opposite directions: In principle, quantum chemistry can deal with strong correlations exactly, but only for small clusters. Thus, finite size effects and the embedding of the clusters have to be controlled. On the other hand, periodic 3D compounds can be calculated reliably in DFT codes, but the correlations are treated in a very approximate manner, often including external parameters like in the widely used LSDA+U method. Using the 1D model compound Li_2CuO_2 as an example, we present a computational study on the DFT level, aiming to a controlled, smooth transition from a 3D system to a cluster while preserving the most relevant physics of the system. Step by step, the structural complexity of the system is reduced, controlling the leading interactions by a tight binding procedure. Our study shall provide deeper insight into the implications caused by the different levels of approximations.

TT 6.25 Mon 13:00 P1A

Magnetic properties of the new low dimensional S=1/2 system: Cu(NO$_3$)$_2$·H$_2$O — M. Yehia[1], E. Vavilova[1,2], •V. Kataev[1], R. Klingeler[1], O. Volkova[3,4], E. Lapsheva[4], V. Shutov[4], O. Savelieva[4], A.N. Vasiliev[4], and B. Büchner[1] — [1]Institute for Solid State Physics, IFW Dresden, 01171 Dresden, Germany. — [2]Kazan Physical Technical Institute, Russian Academy of Sciences, 420029 Kazan, Russia. — [3]Institute of Radiotechnics and Electronics, 125009 Moscow, Russia. — [4]Moscow State University, 119991 Moscow, Russia.

The new low dimensional S=1/2 system $Cu(NO_3)_2·H_2O$ is studied by ESR (9.5 GHz), magnetic susceptibility $\chi(T)$, specific heat $Cp(T)$ and NMR. The anisotropy of the ESR measureables reveals a two dimensional nature of the $Cu^{2+}(S = 1/2)$ layers in this material. The T-dependence of the ESR response for different field directions indicates a substantial magnetic anisotropy and occurrence of different exchange paths in the Cu layers. A phase transition of antiferromagnetic nature at $T_N \sim 3.4$ K can be identified in the $\chi(T)$ data. This is consistent with the specific heat measurements which exhibit a peak at 3.4 K in zero magnetic field. However, an application of an external field of 3 T strongly suppresses this peak. In addition, a broad anomaly has been observed at low temperatures in the $Cp(T)$ data. On the basis of our experimental data we discuss the interplay between the structure and magnetism of this novel compound.

TT 6.26 Mon 13:00 P1A

Surface studies of charge-ordering transition metal oxides by means of scanning tunneling microscopy — Paul Sass[1], •Dirk Bombor[1], Grzegorz Urbanik[1], Torben Hänke[1], Christian Hess[1], Bernd Büchner[1], Pascal Reutler[2], and Alexandre Revcolevschi[2] — [1]Leibniz Institute for Solid State and Materials Research, IFW-Dresden, Germany — [2]Laboratoire de Physico-Chimie de l'Etat Solide, Université Paris Sud, France

The surface of the transition metal oxides $La_{5/3}Sr_{1/3}NiO_4$ and $La_{0.5}Sr_{1.5}MnO_4$ was studied by means of scanning tunneling microscopy (STM). Both materials are model systems for charge ordering phenomena. Despite the insulating nature of these materials we achieved atomic resolution on cleaved surfaces of $La_{5/3}Sr_{1/3}NiO_4$ and $La_{0.5}Sr_{1.5}MnO_4$. Topogrophic images of both compounds reveal periodic modulations, which can be interpreted as signature of short range surface charge ordering. Nevertheless, no direct evidence of charge ordering structures which appear in the volume was found on the surface of our samples. Spectroscopic investigations of the manganite $La_{0,5}Sr_{1,5}MnO_4$ reveal changes in density of states at the fermi level with decreasing temperature, especially an enhacement of the energy gap at the charge ordering temperature.

TT 6.27 Mon 13:00 P1A

Coupled spin S = 1 /2 dimer-systems based on nitronyl-nitroxide biradicals — Cong T. Pham[1], Katarina Removic-Langer[1], •Bernd Wolf[1], Yulia D. Borzdina[2], Evgeny A. Mostovich[2], Martin Baumgarten[2], and Michael Lang[1] — [1]Physikalisches Institut, Universität Frankfurt, SFB/TR49,

60438 Frankfurt(M) — [2]Max-Planck-Institut für Polymerforschung, SFB/TR49, 55128 Mainz

Due to the collective behaviour of their magnetic excitations, arrays of coupled S = 1/2 spin-dimers in magnetic fields are of general interest in solid state physics as they can be considered as a gas of interacting bosons. Depending on whether the repulsion or the hopping of magnetic excitations dominates, the magnons (triplons) may form superlattices or undergo Bose-Einstein condensation (BEC). The investigation of BEC under various conditions, especially the comparison between field- and pressure-induced condensation, as well as the influence of dimensionality is a subject of current interest. In this contribution we will present a new class of coupled spin-dimer systems based on purely organic building blocks. We will show magnetic susceptibility and magnetization data of various nitronyl-nitroxide biradicals from which we extract the influence of the bridging ligands on the intra-dimer coupling constant J. The target materials show moderate values of their intra-dimer exchange coupling and indications for significant inter-dimer couplings. In addition, due to the huge variety of possible bridging ligands and their chemical modification, the magnetic exchange in nitronyl-nitroxide biradicals can be fine tuned.

TT 6.28 Mon 13:00 P1A

Capacitive dilatometry under Helium-gas pressure — •Christian Balz, Andreas Brühl, Rudra Sekhar Manna, Bernd Wolf, and Michael Lang — Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt(M), SFB/TR49, Germany

Important interaction parameters of organic conductors can be tuned by applying moderate external pressure. For the κ-$(ET)_2X$ salts, for instance, many interesting regions of the phase diagram can be traversed by applying pressure of only a few hundred bars (e.g., paramagnetic Mott insulator, antiferromagnetic Mott insulator, superconductor or paramagnetic metal), see, e.g., [1]. Furthermore, thermal expansion measurements have been particularly suitable for exploring phase transitions such as the Mott metal-insulator transition [2], so it is highly desirable to combine the two techniques. In a pilot study, we have performed ultra-high resolution thermal expansion measurements at room temperature and under pressures up to 4 bar by combining capacitive dilatometry with the Helium-gas pressure technique. In a first step, we were able to accurately reproduce the expected pressure-induced changes in the dielectric constant of Helium. In addition, we are assembling a cryostat, where the same type of capacitive dilatometer cell that was used in our pilot experiment will be located inside a pressure cell. With this setup, we target at performing ultra-high resolution thermal expansion ($\Delta l/l \geq 10^{-10}$) measurements over wide ranges of temperatures and hydrostatic Helium-gas pressures up to 2.5 kbar.

[1] S. Lefebvre *et al.*, Phys. Rev. Lett. **85**, 5420 (2000)
[2] M. de Souza *et al.*, Phys. Rev. Lett. **99**, 037003 (2007)

TT 6.29 Mon 13:00 P1A

Magnetic-field dependence of the T^*-anomaly in quasi-2D organic superconductors — Jens Brandenburg[1], •Pintu Das[1], Jens Müller[1,2], Michael Lang[2], Franziska Weickert[1,3], Marek Bartkowiak[3] und Jochen Wosnitza[3] — [1]Max–Planck–Institut für Chemische Physik fester Stoffe, Dresden — [2]Johann–Wolfgang–von–Goethe Universität, SFB/TR49, Frankfurt am Main — [3]Hochfeld–Magnetlabor Dresden, Forschunszentrum Dresden–Rossendorf, Dresden

The family of quasi-2D superconductors $\kappa-(BEDT-TTF)_2X$ are model systems for strongly correlated low–dimensional metals. Recently, the unusual normal–conducting state — characterized by a line of anomalies T^* (in the order of 40 K) — has attracted considerable attention: a "pseudo-gap"behavior in analogy to the high-T_c cuprates, a crossover from an incoherent "bad"metal to a coherent Fermi–liquid regime, and a density–wave–type phase transition have been suggested as possible scenarios. To investigate the possibility of a magnetic origin we carried out detailed transport measurements in pulsed magnetic fields up to 60 T. For two different compounds, X = $Cu[N(CN)_2]Br$ and $Cu(NCS)_2$, we observed a maximum in the relative magnetoresistance change right around T^*. This indicates the significance of magnetic degrees of freedom which are coupled to the transport properties. Also, for the first time we were able to determine the magnetic–field dependence of T^* showing a small negative shift with increasing field. We discuss the implications of our experimental data for possible models explaining the anomalous normal–conducting state.

TT 6.30 Mon 13:00 P1A

Multi-frequency ESR studies on $(TMTTF)_2X$: evidence of the anisotropic Zeeman interaction in the charge ordered state — •S. Yasin[1,2], B. Salameh[2], M. Dumm[2], and M. Dressel[2] — [1]Institut Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [2]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

We studied the charge ordered (CO) state of the quasi 1-D $S = 1/2$ quantum spin chains $(TMTTF)_2X$ (X=SbF_6 and AsF_6) by comprehensive W-Band (95 GHz), Q-band (34 GHz) and X-Band (9.5 GHz) ESR experiments between 4 and 300 K in order to explore the nature of the exchange interaction in the CO state. At high temperatures, both compounds show a linear decrease of the linewidth with decreasing temperature; this behavior does not depend on the applied microwave frequency as well as the anisotropy of both, linewidth and g-value. Below T_{CO}, the breaking of the inversion symmetry of the $(TMTTF)_2$-dimers results in additional contributions ΔH_{CO} to the ESR linewidth. While the linewidth is frequency independent along the three principle magnetic axes a, b', and $c*$, it is substantially enhanced for the Q- and W-band measurements along the diagonal of $a - b'$ plane. The enhanced linewidth along 45^o in the $a - b'$ plane below T_{CO} shows a quadratic frequency dependence which is characteristic for anisotropic Zeeman interaction. From this finding we can conclude that the charge order leads to two inequivalent magnetic sites. We will compare this result to one obtained on anion-ordered TMTTF salts where a different charge-order pattern was proposed.

TT 6.31 Mon 13:00 P1A

Quantum-Phase-Transition within Density Functional Theory using exact Exchange-Correlation Potentials — •Martin Moch[1] and Peter Schmitteckert[1,2] — [1]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D-76021 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

Density Functional Theory (DFT) is one of the most widely used numerical tools to study properties of interacting Fermi systems. In our work we consider the question whether DFT is able to describe the quantum phase transitions based on the interplay of disorder and interaction. To this end we calculate exact Kohn-Sham potentials for disordered, interacting, half-filled, one-dimensional Fermi systems from the local densities obtained from the Density Matrix Renormalization Group (DMRG) calculations. In the framework of Anderson localization one-dimensional systems are always localized. However, for attractive interaction the real system undergoes a phase transition to a metallic phase at a finite interaction. Here we report on the manifestation of this phase transition in the effective non-interacting DFT description.

TT 6.32 Mon 13:00 P1A

Comparison of dynamics in quantum impurity models with bosonic and fermionic baths — •David Roosen[1], Karyn Le Hur[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt/Main, Germany — [2]Department of Physics, Yale University, New Haven, CT 06520, USA

Equivalence relations between quantum impurity models with bosonic and fermionic baths can be derived using the bosonization technique [1]. We focused on the well-known mapping between the anisotropic Kondo and the spin boson model (for a recent review on this model see [2]) and investigated, to which degree this equivalence holds for general local observables, and whether it extends to nonequilibrium dynamics.

The dynamics of the two models are investigated using a time-dependent Numerical Renormalization Group (NRG) algorithm [3] developed recently. A detailed study of the time-dependent entanglement entropy, a measure of increasing importance due to its prominent role in numerous fields of physics ranging from quantum information science to quantum phase transitions in condensed matter systems [4], has been carried out.

[1] S. Chakravarty, Phys. Rev. Lett. **49**, 681 (1982).
[2] K. Le Hur, Annals of Physics **323**, 9, 2208, (2008).
[3] F. Anders, and A. Schiller, Phys. Rev. Lett. **95**, 196801 (2005).
[4] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).

TT 6.33 Mon 13:00 P1A

Dynamical correlation functions in the Ising model with a boundary — •Dirk Schuricht and Fabian H. L. Essler — The Rudolf Peierls Centre for Theoretical Physics, University of Oxford,

United Kingdom

Using scanning tunneling microscopy one can measure the local density of states in the vicinity of impurities. In one-dimensional systems, like stripes in high-temperature superconductors or carbon nanotubes, an impurity is equivalent to a boundary. This motivates the study of correlation functions in models with boundaries. In particular, the low-energy properties of strongly correlated systems are typically described by boundary field theories. We have calculated the dynamical correlation functions in the semi-infinite quantum Ising chain in the presence of a boundary magnetic field [1]. The used form-factor expansion is found to be fastly convergent for $M|R| > 0.1$, where R is the distance from the boundary and $1/M$ the correlation length. At sufficiently late times we observe oscillatory behaviour of the correlations arbitrarily far away from the boundary. We investigate the effects of the boundary bound state that is present for a range of boundary magnetic fields.

[1] D. Schuricht and F. H. L. Essler, J. Stat. Mech.: Theor. Exp. P11004 (2007).

TT 6.34 Mon 13:00 P1A

Quantum Monte Carlo results on phonon softening in the two-dimensional Holstein model — •Prabuddha Chakraborty[1,2], Richard Scalettar[2], and Warren Pickett[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]University of California, Davis, CA 95616, USA

In this poster, we present new observations on the phonon spectral density in the two dimensional Holstein model. The numerical method we use is Determinant quantum Monte Carlo, combined with Maximum Entropy which is used to extract the real frequency spectral density of the phonons. We highlight one of our most surprising observations: the presence of a ubiquitous softening of the phonon at the center of the Brillouin zone, in direct contradiction to established results in this problem. We summarize the behaviour of the softening across a wide range of electron densities, phonon frequencies and electron-phonon interaction strengths.

TT 6.35 Mon 13:00 P1A

Huge thermomagnetic and thermoelectric effects in Luttinger liquids and spin chains — •David Rasch[1], Arti Garg[2], Achim Rosch[1], and Efrat Shimshoni[3] — [1]University of Cologne, Germany — [2]Technion, Haifa, Israel — [3]Bar-Ilan University, Ramat-Gan, Israel

The interplay of Umklapp scattering and weak disorder in Luttinger liquids and spin chains leads to strong effects in the field and doping dependence of transport quantities. We show that the thermal conductivity of spin chains as a function of a magnetic field B displays a pronounced dip for $B \sim T$. In metallic systems, we predict large violations of the Wiedemann Franz law. Depending on the doping, the Wiedemann Franz ratio $\kappa/(\sigma T)$ can become either very large or very small.

TT 6.36 Mon 13:00 P1A

Quantum dots coupled to Luttinger liquid leads - conductance and charging — •Peter Wächter[1], Volker Meden[2], and Kurt Schönhammer[1] — [1]Institut für Theoretische Physik, Universität Göttingen, D-37077 Göttingen — [2]Institut für Theoretische Physik A, RWTH Aachen, D-52056 Aachen

The theoretical description and experimental realization of quantum dots is a very active field in condensed matter physics. In our work, we model quantum dots as non-degenerate energy levels coupled to Luttinger liquid leads, i.e. we couple the zero-dimensional dot to leads of dimension one in order to study how the Luttinger liquid physics in the leads affects the physics of the dot. In particular we identify universal power law scaling in the charging of a single quantum dot and comment on the conductance through such a system. Furthermore we explore the conductance through parallel quantum dots coupled to Luttinger liquid leads.

TT 6.37 Mon 13:00 P1A

Optical signatures of Kondo effect in quantum dots — Hakan E. Türeci[1], Atac Imamoglu[1], Andreas Weichselbaum[2], •Markus Hanl[2], Theresa Hecht[2], and Jan von Delft[2] — [1]Institute of Quantum Electronics, ETH-Zürich, CH-8093 Zürich, Switzerland — [2]Arnold Sommerfeld Center for Theoretical Physics, LMU München, D-80333 München, Germany

We analyze the optical signatures of many body interactions between an optically excited QD electron and an adjacent fermionic reservoir. The optical absorption lineshapes are calculated using the numerical renormalization group, following [1]. The resulting optical lineshape is highly nontrivial: at zero magnetic field, it has a power-law singularity of the form $I(\omega) \sim (\omega - \omega_{th})^{-\sigma}$ with exponent σ showing two distinct cross-overs, which can be understood analytically in terms of the fixed points of the RG flow of the symmetric Anderson model. We also analyze the dependence of the optical response on external magnetic field and finite temperature.

[1] R. Helmes et al., Phys. Rev. B, **72**, 125301 (2005)

TT 6.38 Mon 13:00 P1A

Superperturbation solver for quantum impurity models — •Christoph Jung[1], Hartmut Hafermann[1], Sergey Brener[1], Mikhail Katsnelson[2], Alexei Rubtsov[3], and Alexander Lichtenstein[1] — [1]I. Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Institute for Molecules and Materials, Radboud University of Nijmegen, 6525 AJ Nijmegen, The Netherlands — [3]Department of Physics, Moscow State University, 119992 Moscow, Russia

We present a very efficient solver for the general Anderson impurity problem. It is based on the perturbation around a solution obtained from exact diagonalization using a small number of bath sites. We formulate a perturbation theory which is valid for both weak and strong coupling and interpolates between these limits. Good agreement with numerically exact quantum Monte-Carlo results is found for a single bath site over a wide range of parameters. In particular, the Kondo resonance in the intermediate coupling regime is well reproduced for a single bath site and the lowest order correction. The method works directly on the real axis and thus allows to access the density of states without the need of analytical continuation of imaginary time data.

TT 6.39 Mon 13:00 P1A

Comparison between NRG and DMRG as impurity solver — •Robert Peters, Piet Dargel, and Thomas Pruschke — Friedrich Hund Platz 1, 37077 Goettingen

Impurity models like the Anderson model play an important part in strong correlation physics. They model the situation of localized, partially filled f- or d-shells in metals and artificially produced quantum dots or Qubits. Also strongly correlated lattice models, like e.g. the Hubbard model, can be mapped via dynamical mean field theory on a self-consistency calculation of an impurity model. In recent years the Density Matrix Renormalization Group (DMRG) was introduced as novel method to solve such impurity problems. We here compare results for static and dynamic properties of quantum impurities obtained with DMRG to those from the well-established Numerical Renormalization Group (NRG). Special emphasis will be put on the possible application of DMRG to systems with multiple orbitals or multiple impurities.

TT 6.40 Mon 13:00 P1A

Kondo model in and out of equilibrium: Functional RG at strong coupling — •Holger Schmidt and Peter Wölfle — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D-76128 Karlsruhe, Germany

We apply the functional renormalization group (RG) method to calculate the conductance of a quantum dot in the Kondo regime in and out of equilibrium. The local spin 1/2 operator is described in pseudofermion representation. The set of of coupled RG equations for the pseudofermion self-energy and vertex functions in Keldysh space is derived and analyzed. Neglecting three-particle and higher vertex functions the equations are solved. It is found that the imaginary part of the self energy limits the growth of the two-particle vertex function at low temperatures and voltages $T, V \ll T_K$ (Kondo temperature), providing a semiquantitative description down into the strong coupling regime. In the regime $\max(T, V) \gg T_K$ we recover the results of [1].

[1] A. Rosch *et al.*, Phys. Rev. Lett. **90**, 076804 (2003).
[2] J. Paaske *et al.*, Phys. Rev. B, **70**, 1553041 (2004).

TT 6.41 Mon 13:00 P1A

Correlation effects in the two-site Anderson model (TIAM) — •Torben Jabben — TU-Darmstadt, Darmstadt, Hessen

Within the framework of the enhanced non-crossing approximation (ENCA), an approximative solution of the TIAM is obtained, which is applicable to any finite value of the Coulomb repulsion U.

One-particle spectra and thermodynamic properties are presented

and discussed. Especially the competition between two independent Kondo effects at each impurity and the non-local singlet or triplet formation between both impurities is discussed.

TT 6.42 Mon 13:00 P1A

Variational local moment approach to Kondo effect in the multi-orbital Anderson impurity model — •Anna Kauch[1] and Krzysztof Byczuk[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Institute of Theoretical Physics, Faculty of Physics, Warsaw University, Hoza 69, PL-00-681 Warszawa, Poland

The recently developed [1,2] variational local moment approach (VLMA) to the single impurity Anderson model is presented. We focus on the application of the method to the multi-orbital impurity model in various regions of parameters where different types of Kondo effects can occur. The application of VLMA to the multi-orbital Hubbard model as an impurity solver of the dynamical mean-field theory equations is also addressed.

The method is based on assuming the existence of local moments – following the single orbital local moment approach of D. Logan [3]. The values of the local moments are obtained within VLMA by minimizing the ground state energy of the system.

[1] A. Kauch and K. Byczuk, Physica B 378-380, 297 (2006).

[2] A. Kauch and K. Byczuk, Quantum Magnetism, Proceedings of the NATO Advanced Study Institute on Quantum Magnetism, Les Houches, France, pp. 85-95 (Springer, 2008).

[3] D. Logan and M.T. Glossop, J. Phys. Condens. Matter 12, 985 (2000).

TT 6.43 Mon 13:00 P1A

Kondo screening cloud in the Anderson impurity model — •Andreas Holzner[1,2], Fabian Heidrich-Meisner[1], Ian McCulloch[3], Ulrich Schollwöck[1], and Jan von Delft[2] — [1]Institut für Theoretische Physik C, RWTH Aachen University, D-52056 Aachen, Germany — [2]Lehrstuhl für Theoretische Festkörperphysik, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany — [3]School of Physical Sciences, University of Queensland, QLD 4072, Australia

A magnetic moment in a metal or in a quantum dot is, at low temperatures, screened by the conduction electrons by the mechanism of the Kondo effect. This gives rise to spin-spin correlations between the magnetic moment and the conduction electrons, which can have a substantial spatial extension. We study this phenomenon, the so-called Kondo cloud, by means of the density matrix renormalization group method for the case of the single-impurity Anderson model. Our goal is to elucidate whether the Kondo screening length, typically assumed to be proportional to the inverse Kondo temperature, can be extracted from the spin correlations. For several mechanisms that destroy the Kondo effect, we investigate the induced behavior of the screening cloud.

TT 6.44 Mon 13:00 P1A

The chaotic Kondo box: mean-field approach — •Sebastien Burdin[1], Rainer Bedrich[2], and Martina Hentschel[2] — [1]Institute of Theoretical Physics, Cologne University — [2]Max Planck Institute for the Physics of Complex Systems, Dresden

We study the low temperature physical properties of a mesoscopic bath of electrons (E.g., a big quantum dot), coupled to a local Kondo impurity (E.g., a small quantum dot, or a magnetic ion). Here, a crucial difference with the Kondo effect occuring in a bulk material results from a finite mean level spacing. This low energy scale can generate deviations from the universal behavior which would be expected for a bulk system. Using a mean-field approximation for the Kondo interaction, we consider as a first step a "clean system", where the non-interacting energy levels are characterized by a constant distribution. Then, a more realistic situation is considered, for which the energy levels are distributed randomly. This is realized within the random matrix theory. In both cases, we study the local magnetic susceptibility, the conductance, and the local density of electronic states as a function of the temperature, the mean level spacing, the Kondo coupling, and the number of electrons on the dot.

TT 6.45 Mon 13:00 P1A

Periodic time dependent Kondo model — Markus Heyl and •Stefan Kehrein — Arnold-Sommerfeld-Center for Theoretical Physics, Ludwigs-Maximilians-Universität München

In this work we study a nonequilibrium steady state in the Kondo model generated by periodic switching of the interaction. As has been shown in Ref. [1], at the Toulouse point the Kondo model can be mapped onto a noninteracting resonant level model even for nonequilibrium interaction quenches. Since the resonant level model is exactly solvable, we are therefore able to investigate the real-time dynamics on all time scales, especially the buildup of the steady state. We characterize this steady state by calculating the spin-spin correlation function.

[1] D. Lobaskin and S. Kehrein, J. Stat. Phys. **123**, 301-313 (2006).

TT 6.46 Mon 13:00 P1A

Continuous-Time Quantum Monte Carlo Approach to Strongly Correlated Nonlinear Transport — •Andreas Dirks[1], Thomas Pruschke[1], and Philipp Werner[2] — [1]Institut für Theoretische Physik, Universität Göttingen — [2]Institut für Theoretische Physik, ETH Zürich

The tremendous progress in nano structuring made a broad variety of physical phenomena of quantum impurity systems experimentally accessible through transport measurements. However, computational methods for a reliable description of strongly correlated transport are still rare. We investigate the application of continuous-time Quantum Monte Carlo algorithms to the imaginary-time formalism introduced by Han and Heary [1].

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

TT 6.47 Mon 13:00 P1A

Uniaxial pressure effects on the superconductivity of $CeCoIn_5$ — •Kai Grube[1], Sebastian Zaum[1,2], Roland Schäfer[1], Eric D. Bauer[3], Christoph Meingast[1], and Hilbert v. Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [3]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

The heavy-fermion superconductor $CeCoIn_5$ shows strongly anisotropy thermodynamic and transport properties due to its tetragonal crystal structure. A comparison with its cubic parent compound $CeIn_3$, with an order of magnitude smaller transition temperature T_c, suggests the importance of anisotropy for the superconducting pairing mechanism in these alloys. We have performed thermal expansion and magnetostriction measurements along the a- and c-axes of $CeCoIn_5$ single crystals. From measurements transverse and longitudinal to magnetic fields up to $B = 14\,\mathrm{T}$, it has been possible to calculate the uniaxial pressure effects on the superconductivity, dT_c/dp_i ($i = a$, c) and dB_{c2}/dp_i, and the Grüneisen parameters, $\Gamma_a(T, B)$ and $\Gamma_c(T, B)$. We will discuss the stress and strain dependences of the characteristic energy scales and relate them to the effects of hydrostatic pressure, magnetic field, and doping.

TT 6.48 Mon 13:00 P1A

Coexistence of antiferromagnetism and superconductivity in Cd-doped $CeCoIn_5$ — •O. Stockert[1], U. Witte[2,3], M. Nicklas[1], R. Schedler[3], K. Kiefer[3], J. D. Thompson[4], A. D. Bianchi[5], Z. Fisk[5], and F. Steglich[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [4]Los Alamos National Laboratory, Los Alamos NM, USA — [5]University of California, Irvine CA, USA

Starting from the heavy-fermion superconductor $CeCoIn_5$ with a superconducting $T_c = 2.3\,\mathrm{K}$, doping with cadmium induces antiferromagnetic order in $CeCo(In_{1-x}Cd_x)_5$ above a critical Cd concentration $x_c \approx 0.005$ with a subtle interplay between magnetism and antiferromagnetism. We report on elastic neutron scattering experiments of the heavy-fermion alloy $CeCo(In_{1-x}Cd_x)_5$ with $x = 0.0075$ to study the magnetic structure and the influence of superconductivity on the antiferromagnetism. Below $T_N = 2.4\,\mathrm{K}$ and down to lowest temperatures $T < 100\,\mathrm{mK}$ commensurate antiferromagnetic order with a propagation vector $\tau = (1/2\ 1/2\ 1/2)$ was detected. The transition into the superconducting state at $T_c = 1.7\,\mathrm{K}$ is accompanied by a kink in the magnetic intensity followed by a saturation towards lower temperatures at a reduced value. These results indicate a coexistence of antiferromagnetism and superconductivity, but reveal at the same time a strong influence of the superconducting state on the magnetic order. Our results will be discussed in comparison to other heavy-fermion superconductors.

TT 6.49 Mon 13:00 P1A

Scanning Tunneling Spectroscopy studies on heavy fermion superconductors — •Stefan Ernst[1], Steffen Wirth[1], Hirale Jeevan[1], Christoph Geibel[1], Frank Steglich[1], and Zachary Fisk[2] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]Department of Physics and Astronomy, UC Irvine, USA

Scanning Tunneling Spectroscopy (STS) is a powerful tool for mapping the local electronic density of states (DOS) of sample surfaces. Of particular interest are experiments with superconducting (SC) materials, as information about the SC energy gap can directly be obtained. The application of STS to heavy fermion (HF) superconductors might be a valuable contribution to the understanding of this class of materials. Fundamental properties such as the symmetry of the SC order parameter or excitations due to the SC pairing interaction might be revealed.

This work reports on STM measurements carried out at low temperatures and under ultra-high vacuum (UHV) conditions with the possibility of applying a magnetic field. For the materials investigated here, spectroscopic features in the order of a few hundred μeV are expected. The sufficiently high resolution of our STM, in particular with respect to energy, has been verified. Due to the short SC coherence length of HF materials, a clean tunnel junction is required to investigate the SC gap by means of STS. Methods were developed to prepare clean surfaces of single crystals *in situ*. Preliminary STM and STS measurements were conducted on single crystalline samples of the HF superconductors $CeCoIn_5$, $CeIrIn_5$, and $CeCu_2Si_2$.

TT 6.50 Mon 13:00 P1A

Magnetic field dependency of the spin wave excitation gap in UPt_2Si_2 — •Dirk Schulze Grachtrup[1], Matthias Bleckmann[1], Stefan Süllow[1], and John A. Mydosh[2] — [1]TU Braunschweig, Institute for Physics of Condensed Matter, Mendelssohnstr. 3, 38106 Braunschweig, Germany — [2]University Cologne, II. Physikalisches Institut, Zülpicher Str. 77, 50937 Cologne, Germany

Tetragonal UPt_2Si_2 has recently been characterized as moderately mass enhanced antiferromagnetic compound, which in various physical properties reveals a resemblance to the hidden order material URu_2Si_2 [1,2].

To further characterize this resemblance we have examined UPt_2Si_2 with resistivity measurements in magnetic fields. In particular, we find the antiferromagnetic phase transition at T_N=32 K in zero field to shift slightly downwards to 31 K at B = 9 T // c-axis. Further, the temperature dependence of the resistivity in the range up to 20K can be described by an opening of a spin wave excitation gap. In contrast to T_N this gap displays a much larger reduction by about 30% with increasing magnetic field up to 9T. We discuss the relationship between spin excitation gap and magnetic ordering, this in particular with respect to the difference in field response.

[1] S. Süllow, A. Otop, A. Loose, J. Klenke, O. Prokhnenko, R. Feyerherm, R.W.A. Hendrikx, J.A. Mydosh, H. Amitsuka, J. Phys. Soc. Jpn. **77** (2008) 024708
[2] N. Johannsen, S. Süllow, A.V. Sologubenko, T. Lorenz, J.A. Mydosh, Phys. Rev. B **78** (2008) 121103

TT 6.51 Mon 13:00 P1A

Interplay between crystal-field splitting and Kondo-effect in $CeNi_9Ge_{4-x}Si_x$. — Christian Gold[1], Ludwig Peyker[1], •Ernst-Wilhelm Scheidt[1], Wolfgang Scherer[1], and Herwig Michor[2] — [1]Institut für Physik, Universität Augsburg, 86159 Augsburg, Germany — [2]Institut für Festkörperphysik, TU Wien, 1040 Wien, Austria

$CeNi_9Ge_4$ exhibits a Kondo lattice behavior with unusual single-ion non-Fermi-lquid features and with the largest ever recorded value of the electronic specific heat $\Delta C/T \approx 5.5\,\mathrm{J/mol\,K^2}$ without showing any trace of magnetic order. An entropy calculation yielding $S = Rln4$ at $T < 20\,\mathrm{K}$ suggests that in $CeNi_9Ge_4$ a crystal electrical field (CEF) ground state quasi quartet of Ce^{3+} splits into two doublets leading to an interplay between Kondo effect and CEF splitting on the same energy scale. $CeNi_9Si_4$ is a Kondo lattice system with an enhanced Sommerfeld coefficient of $\gamma \approx 155\,\mathrm{mJ/mol\,K^2}$ which can be well described by the degenerate Coqblin-Schrieffer model ($J = 5/2$). Here we report on specific heat, susceptibility and resistivity measurements of the substitution series $CeNi_9Ge_{4-x}Si_x$ which *i*) exhibits a continuous crossover from a four-folder CEF ground state to a two folder one in present of Kondo screening for $x = 0.5$ - 4 and which *ii*) follows a reduction of the Kondo temperature T_K with decreasing lattice volume between $x = 0$ and 0.1, which is in contrast to the compressible Kondo lattice model.

TT 6.52 Mon 13:00 P1A

Polarization dependent XAS on $CeMIn_5$ (M=Co, Rh and Ir) and $CePt_3Si$ determines crystal-field ground state and sequence of states. — •T. Willers[1], A. Severing[1], Z. Hu[1], N. Hollmann[1], P.O. Körner[1], H.-J. Lin[2], C.T. Chen[2], D. Schmitz[3], E.D. Bauer[4], B. Fak[5], G. Lapertot[5], and L.H. Tjeng[1] — [1]Institute of Physics II, University of Cologne — [2]NSRRC, Taiwan — [3]BESSY, Berlin — [4]Los Alamos Nat. Lab., Los Alamos, NM, USA — [5]CEA, SPSMS, Grenoble, France

The tetragonal compounds $CeMIn_5$ (P4/mmm) are of interest since the interplay between the antiferromagnetic behaviour of the Ce local moments, an unconventional normal state, and superconducting behaviour of the heavy electrons can be studied [1 and references therein]. The non-centro symmetric system $CePt_3Si$ is also tetragonal (P4/mm), becomes antiferromagnetic at 1K and superconducting below 0.7K [2]. In all these compounds the knowledge of the crystal-field potential is crucial for the description of the low temperature properties. Here linear polarized soft X ray absorption data at the Ce-M_{45} edges of $CeMIn_5$ with M=Co, Rh and Ir and $CePt_3Si$ will be presented with the view to elucidate the crystal field schemes of these compounds. Not only the ground state symmetry, but also the sequence of states could be obtained from the temperature dependence of the XAS data. Furthermore the influence of the Kondo effect on the Ce-M_{45} edges of these compounds will be discussed.

[1] J.L. Sarrao and J.D. Thompson, J. Phys. Soc. Japan **76,** 051013 (2007). [2] E. Bauer et al., Physica B **359,** 360 (2005).

TT 6.53 Mon 13:00 P1A

Ge based filled skutterudites MPt_4Ge_{12}: a ^{195}Pt NMR study. — •M. Baenitz, R. Sarkar, R. Gumenik, A. Leithe-Jasper, W. Schnelle, H. Rosner, U. Burkhardt, M. Schmidt, U. Schwarz, Yu. Grin, and F. Steglich — Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

Filled skutterudites MT_4X_{12}(M: alkaline or rare earth metals, T: Fe, Ru, Os, X: P, As, Sb) show a wide variety of strongly correlated electron physics from heavy fermions to Kondo insulators to unconventional superconductors. The new type of skutterudites, the Ge based system MPt_4Ge_{12} form with M = Ba, Sr, La, Ce, Pr, Sm, Eu[1,2]. They exhibit metallic behaviour and show, with the exception of the systems with Ce, Sm and Eu, superconductivity at low temperature (T_c < 10 K)[1,2]. Here we present a temperature dependent ^{195}Pt NMR study on the whole series of MPt_4Ge_{12} compounds with special attention on the magnetic systems with Ce, Sm and Eu. Here shift ^{195}K(T) and spin lattice relaxation rate are discussed in the context of a dense Kondo system with a mixed valence state of Ce as well as for Sm. Especially the pronounced maximum observed in ^{195}K(T) provides very strong evidence for a mixed valence behavior for this new class of material.

[1] Phys. Rev. Lett. 100, 017002 (2008).
[2] Phys. Rev. Lett. 99, 217001 (2007).

TT 6.54 Mon 13:00 P1A

Possible crystal electrical field shift in the system $CeNi_{9-x}Cu_xGe_4$. — •Ernst-Wilhelm Scheidt[1], Ludwig Peyker[1], Christian Gold[1], Wolfgang Scherer[1], Ernst Bauer[2], Herwig Michor[2], Tobias Unruh[3], and Peter Link[3] — [1]Institut für Physik, Universität Augsburg, 86159 Augsburg, Germany — [2]Institut für Festkörperphysik, TU Wien, 1040 Wien, Austria — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz, Technische Universität München, 85747 Garching, Germany

Crystal structure, specific heat, magnetic susceptibility, electrical resistivity and inelastic neutron studies on the heavy fermion system $CeNi_{9-x}Cu_xGe_4$ ($0 \le x \le 1$) reveal a continuous tuning of the ground state by Ni/Cu substitution from an effectively fourfold degenerate non-magnetic Kondo ground state of $CeNi_9Ge_4$ with pronounced non-Fermi-liquid (nFL) features towards a magnetically ordered, effectively twofold degenerate ground state in $CeNi_8CuGe_4$ with $T_N = 0.18\,\mathrm{K}$. NFL behavior, $C/T \propto \chi \propto -\ln T$ and $\rho \propto T$, is observed for $x \cong 0.4$. Hitherto, this is the first example where a substitution driven quantum phase transition is connected not only with changes of the relative strength of Kondo effect and RKKY interaction, but also with a reduction of the effective crystal field ground state degeneracy.

TT 6.55 Mon 13:00 P1A

Low-temperature specific heat of the heavy-fermion su-

perconductor $CeCu_2Si_2$ — •Julia Arndt[1], Oliver Stockert[1], Robert Borth[1], Thomas Lühmann[1], Hirale Jeevan[1,2], Christoph Geibel[1], Michael Loewenhaupt[3], and Frank Steglich[1] — [1]Max-Planck-Institut f. Chem. Physik fester Stoffe, Dresden — [2]I. Physikal. Inst., U Göttingen — [3]Inst. f. Festkörperphysik, TU Dresden

$CeCu_2Si_2$, the first heavy-fermion superconductor to be discovered, exhibits a complex interplay of antiferromagnetism and superconductivity (SC). In very subtle dependence on the exact stoichiometry its ground state is either antiferromagnetically ordered (A-type), superconducting (S-type), or both (A/S-type). Recent neutron scattering experiments on S-type $CeCu_2Si_2$ ($T_c \approx 600$ mK) [1] and their theoretical interpretation [2] give indications of magnetically mediated SC with an order parameter of $d_{x^2-y^2}$ symmetry. Different order parameter symmetries cause characteristic temperature dependences of the specific heat well below T_c. We performed measurements of the specific heat at temperatures from 50 mK to 4 K and magnetic fields up to 8 T on large single crystals of A-, S- and A/S-type $CeCu_2Si_2$ as well as on 2% and 10% Ge doped $CeCu_2Si_2$ using an adapted quasi-adiabatic heat-pulse method with background heating. The results are compared with each other, with special focus given to the analysis of the low-temperature specific heat of S-type $CeCu_2Si_2$ in order to be able to draw conclusions as to the nature of SC in the system.

[1] O. Stockert *et al.*, Physica B **403**, 973 (2008)
[2] I. Eremin *et al.*, Phys. Rev. Lett. **101**, 187001 (2008)

TT 6.56 Mon 13:00 P1A

Boron-induced change of valence state of Eu and structural phase transition in $EuPd_3B_x$ ($0 \leq x \leq 0.55$) — •Roman Gumeniuk, Claire Loison, Walter Schnelle, Wilder Carrillo-Cabrera, Paul Simon, Ulrich Burkhardt, Marcus Schmidt, Miriam Schmitt, Ulrich Schwarz, Helge Rosner, and Andreas Leithe-Jasper — MPI für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

A detailed experimental and theoretical study of the solubility of B in $EuPd_3$ ($AuCu_3$ structure type) and its influence on the physical properties is presented. 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 $x > 0.2$ together with an anomaly in the unit cell volume. At 950 °C the incorporation of B in $EuPd_3B_x$ is possible up to $x = 0.55$, as can be concluded from the lattice parameters, WDXS and chemical analyses. Transmission electron microscopy investigations show the existence of a superstructure for $Eu_2Pd_6B_y$ in the region of $0.7 \leq y \leq 1$ (Ti_2Rh_6B structure type [1], space group $Fm\bar{3}m$, $a = 8.3096(2)$-$8.3730(2)$ Å). From Eu L_{III} XAS studies as well as from magnetic susceptibility data it can be deduced that the Eu species in $EuPd_3$ and in $EuPd_3B_x$ ($0 \leq x \leq 0.2$) exhibit a $4f^6$ state, while for $EuPd_3B_x$ ($0.2 \leq x \leq 0.35$) and $Eu_2Pd_6B_y$ ($0.7 \leq y \leq 1$) they are in an intermediate valence state. Our findings are discussed with respect to previously published studies [2,3].

[1] B. Fowka *et al.* Z. Krist. 221 (2006) 445.
[2] B. Darshan *et al.* Phys. Rev. B, 30 (1984) 4031.
[3] S.K. Dhar *et al.* Phys. Rev. B, 29 (1984) 5953.

TT 6.57 Mon 13:00 P1A

^{11}B NMR study of the low dimensional Kondo lattice $YbNiB_4$ — •Rajib Sarkar[1], Michael Baenitz[1], Arpana Prasad[2], Zakir Hossain[2], Frank Steglich[1], and Cristoph Geibel[1] — [1]Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Physics, Indian Institute of Technology, Kanpur 208016, India

$YbNiB_4$ deserves special attention because of its interesting physical properties. Recently we reported $YbNiB_4$ being a Kondo system with a strong 2D character, which makes this compound unique among the Yb-based systems. Two antiferromagnetic transitions show up at 5.4 K and 4.0 K [1]. Furthermore the structural homologue $YbAlB_4$ is proposed to be a heavy Fermion system showing superconductivity at T_c=80 mK and quantum criticality without external tuning [2]. Here we present for the first time ^{11}B NMR results on $YbNiB_4$ as a function of temperature (2-295 K) and field. ^{11}B NMR spectra are typical powder pattern with pronounce first order quadrupolar splitting. By lowering the temperature spectra is shifted and broadened. The observed small negative shift indicates the relevance of conduction electron polarization by the Yb $4f^{13}$ moments. Further analysis of shift as well as the spin-lattice relaxation is in progress.

[1] A. Prasad et. al., to be published,
[2] Nature Physics 4, 603(2008).

TT 6.58 Mon 13:00 P1A

Strong electron correlations in $FeSb_2$: An optical investigation and comparison with $RuSb_2$ — •Alexander Herzog[1], Michael Marutzky[1], Jörg Sichelschmidt[1], Anders Bentien[1], Frank Steglich[1], Shin-Ichi Kimura[2], Simon Johnsen[3], and Bo Iversen[3] — [1]MPI Chemical Physics of Solids, 01187 Dresden, Germany — [2]UVSOR, Institute for Molecular Science, Okazaki 444-8585, Japan — [3]Dep. of Chemistry, University of Aarhus, 8000 Aarhus, Denmark

We investigated the far-infrared optical conductivity of $FeSb_2$, being a possible d electron Kondo semiconductor, and its non magnetic homologue $RuSb_2$. For $FeSb_2$ we found an indirect gap of 30 meV and semiconducting behavior for all crystal axes. Another gap feature at 6 meV, appearing below $T = 100$ K, possibly corresponds to the colossal Seebeck coefficient [1] and may therefore be related to strong electronic correlations. However, we found a clear decrease of the reflectivity around 6 meV upon applying a magnetic field which demonstrates contradictory behavior to a common Kondo semiconductor scenario. We propose multiple absorptions due to disordered Fe atoms to be the origin of this gap feature. Furthermore, we discuss a possible relation of an anomalous change in the phonon spectrum of $RuSb_2$ below 100 K to the opening of a 6 meV gap in the isostructural $FeSb_2$. Nevertheless, strong electronic correlations are indicated by a temperature dependent spectral weight redistribution up to energies as large as 1 eV.

[1] A. Bentien et al., Europhys. Lett. **80**, 39901 (2007).

TT 6.59 Mon 13:00 P1A

^{121,123} Sb magnetic resonance as a local probe for gap formation in $FeSb_2$ — •Michael Baenitz[1], Andrei Gippius[2], Simon Johnsen[3], Bo Iversen[3], and Frank Steglich[3] — [1]Max-Planck Institut for Chemical Physics of Solids, Dresden, Germany — [2]Faculty of Physics, Moscow State University, Moscow, Russia — [3]Department of Chemistry, University of Aarhus, Denmark

There is a revived interest on $FeSb_2$ after classifying this system as the second Fe containing Kondo insulator after FeSi. The formation of a spin and charge gap out of an enhanced density of states $N(E_F)$ is one of the key features of these materials. Furthermore $FeSb_2$ surprisingly shows a colossal Seebeck coefficient around 10 K. Here we report on a comparative study on $FeSb_2$ and its structural homologue $RuSb_2$. For both compounds we found two regimes in the temperature dependence of $^{123}(1/T_1)$. Above 40 K (HT) a conventional activated behavior (with D/k_B @ 450 K for $FeSb_2$) dominates in $1/T_1$. Below 40 K (LT) in both systems an unconventional $1/T_1$ behavior with a smooth maximum at 10 K is observed. To analyze this behavior we propose the presence of T-dependent in-gap states forming a narrow band of localized spins with S = 1/2 near the bottom of the conduction band. This model enables us to fit the $^{123}(1/T_1)$ data in the entire temperature range (LT + HT) for $FeSb_2$. Furthermore the relevance of these in-gap states for the colossal Seebeck effect is discussed.

TT 6.60 Mon 13:00 P1A

Quantum phase transition of the sub-Ohmic spin-boson model — •André Winter and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, PF 151150, D-66041 Saarbrücken

Quantum dissipation plays a highly interesting role in several fields of physics, like the decoherence of qubits or charge transfer in donor-acceptor systems. Therefore, we study these quantum-dissipative effects via the spin-boson model, which describes a two-level system coupled to a bosonic bath with a spectral density $J(\omega) \propto \omega^\sigma$. We use an advanced Monte Carlo cluster algorithm to explore the quantum phase transition between localized and delocalized phase of this model in the sub-Ohmic regime ($0 < \sigma < 1$). The applied method, which based on the path integral approach to Quantum Monte-Carlo computations, works without discretization and uses cluster updates of continuous worldline-segments to investigate the quantum critical point effectively. We compute the critical exponents of the phase transition and their dependence on the bath exponent characterizing the low frequency behaviour of the spectral function of the bosonic bath.

TT 6.61 Mon 13:00 P1A

Longitudinal magnon decay near a quantum critical point — •Lucas Hollender and Matthias Vojta — Institut für theoretische Physik, Universiät zu Köln, Köln, Deutschland

A spin dimer system shows a zero-field magnetic order-disorder transition at a critical ratio of the inter-dimer to intra-dimer couplings.

We investigate the decay process of the longitudinal magnon in the antiferromagnetic phase, which has been observed in neutron scattering experiments, as function of the distance to the quantum phase transition. We employ a perturbative analysis within a modified bond operator formalism to compute the lifetime of the longitudinal mode and compare the results to recent neutron scattering measurements on $TlCuCl_3$.

TT 6.62 Mon 13:00 P1A

A 'hidden disorder' scenario for the low-temperature phase transitions in heavy-fermion compounds — •Tanja Rindler-Daller and Matthias Vojta — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

In the study of the low-temperature phase transitions in heavy-fermion compounds, one encounters a complex variety of ordering phenomena. In particular, the nature of the so-called 'hidden order' transition in URu_2Si_2, which is characterized by severe thermodynamical signatures, is not yet fully understood. We adopt an effective theory with 2 competing fields in order to explore the idea of 'hidden disorder'. By performing a scaling analysis and studying a simple model, we can show that the proposed scenario is able to account for the observed anomalies in the specific heat, and serves thus as a rationale for a more detailed microscopic analysis, which is under way.

TT 6.63 Mon 13:00 P1A

Quantum Criticality of the Pomeranchuk Instability: Interplay of Multiple Dynamical Exponents — •Mario Zacharias[1], Markus Garst[1], Achim Rosch[1], and Peter Wölfle[2] — [1]Institut für Theoretische Physik, Universität zu Köln — [2]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe

We consider the Pomeranchuk instability of an isotropic Fermi liquid in two dimensions, $d = 2$. The effective Ginzburg-Landau theory contains two critical modes with different dynamics. There is a ballistic mode with dynamical exponent $z = 2$ and a Landau-damped mode with $z = 3$. While the $z = 3$ mode dominates thermodynamics at $T > 0$ the $T = 0$ quantum dynamics is governed by the $z = 2$ mode. As the $T = 0$ theory is at its upper critical dimension we use the renormalization group (RG) to analyse the leading logarithmic singularities. The resulting universality class is found to be distinct from the Ising- as well as from the XY-model.

At finite temperatures, there is an intricate interplay between the two modes. At criticality, the length scales $\xi_T \sim T^{-1/z}$ separates the quantum from the classical regime. The different dynamical exponents yield an overlap regime where the ballistic mode still has its quantum character while the damped mode is already classical. We find that this regime dominates the properties at finite T. In particular, we argue that the usual separation of quantum and classical dynamics at $T > 0$ is not valid, implying a breakdown of "dimensional reduction". Further, this interplay leads to a universal T dependence of the correlation length at criticality.

TT 6.64 Mon 13:00 P1A

Emergent Lorentz symmetry with vanishing velocity in a critical two-subband quantum wire — •Matthias Sitte[1], Achim Rosch[1], Julia S. Meyer[2], Konstantin A. Matveev[3], and Markus Garst[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA — [3]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

We consider a quantum wire with two subbands of spin-polarized electrons in the presence of strong interactions. We focus on the quantum phase transition when the second subbands starts to get filled. Performing a one-loop renormalization group (RG) analysis of the effective Hamiltonian, we identify the critical theory as a conformal field theory (CFT) of three Majorana fields having an enhanced SU(2) symmetry and central charge $c = 3/2$. While the fixed point is Lorentz invariant, the effective velocities vanish at low energies due to marginally irrelevant operators leading to, e.g., a diverging critical specific heat coefficient. This behavior should occur quite generally in systems where marginally irrelevant terms in the Hamiltonian break Lorentz invariance.

[1] M. Sitte, A. Rosch, J. S. Meyer, K. A. Matveev, and M. Garst, (arXiv:cond-mat/0811.4579).

TT 6.65 Mon 13:00 P1A

Thermal Expansion and Heat Transport of low-dimensional Magnetic Systems close to Quantum Criticality — •Jens Rohrkamp[1], Thomas Lorenz[1], Alexandr Sologubenko[1], Oliver Heyer[1], Markus Garst[2], Fabrizio Anfuso[2], Achim Rosch[2], Karl Krämer[3], and Mark Turnbull[4] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Theoretische Physik, Universität zu Köln — [3]Department of Chemistry and Biochemistry, University of Bern — [4]Carlson School of Chemistry and Department of Physics, Clark University

Compounds with magnetic subsystems representing simple model spin systems with weak magnetic coupling constants are ideal candidates to test theoretical predictions for the generic behavior close to quantum phase transitions. We present measurements of the thermal expansion, magnetostriction and thermal conductivity of the spin-$\frac{1}{2}$-ladder system piperidinium copper bromide $(C_5H_{12}N)_2CuBr_4$ and the spin-$\frac{1}{2}$-chain compound copper pyrazine dinitrate $Cu(C_4H_4N_2)(NO_3)_2$. Both compounds show quantum phase transitions as a function of magnetic field with pressure dependent critical fields. The low-temperature thermal expansion approaches $1/\sqrt{T}$ divergences at the critical fields and shows a complex behavior with various sign changes inbetween.

TT 6.66 Mon 13:00 P1A

Quantum evolution from spin-gap to antiferromagnetic state in the frustrated J_1-J_2 system $(CuCl_{1-x}Br_x)La(Nb_{1-y}Ta_y)_2O_7$ — •Vladimir Gnezdilov[1,2], Peter Lemmens[2], Kwang-Yong Choi[3], and Hiroshi Kageyama[4] — [1]ILTP, Kharkov, Ukraine — [2]IPKM, TU Braunschweig, Germany — [3]Chung-Ang Univ., Seoul, Korea — [4]IC Kyoto, Japan

The $(CuCl_{1-x}Br_x)La(Nb_{1-y}Ta_y)_2O_7$ frustrated system shows a quantum evolution from a spin-gap to an antiferromagnetic state [1] depending on composition x and y. Pronounced effects are observed in Raman spectra in dependence of x and y. Taking into account all previous experimental observations and models, our Raman data are used to identify a realistic coordinate environment of Cu^{2+} ions in the CuCl layers. Work supported by DFG and ESF-HFM.

[1]. Y. J. Uemyra et al., arXiv:0806.2021v1.

TT 6.67 Mon 13:00 P1A

Low frequency spin dynamics in the S=1/2 Heisenberg chain compound $Cu(C_4H_4N_2)(NO_3)_2$ (CuPzN) measured by ^{13}C- and ^{14}N-NMR spectroscopy — •M. Günther[1], H. Kühne[1,2], H.-H. Klauss[1], M. Falkner[2], J. Litterst[2], S. Grossjohann[3], W. Brenig[3], A.P. Reyes[4], P.L. Kuhns[4], C.P. Landee[5], and M.M. Turnbull[5] — [1]IFP, TU Dresden — [2]IPKM, TU Braunschweig — [3]ITHP, TU Braunschweig — [4]NHMFL, FSU, USA — [5]DPC, Clark University, USA

The local magnetization and low frequency magnetic dynamics of the antiferromagnetic S=1/2 Heisenberg chain compound CuPzN have been explored both theoretically and experimentally by means of ^{13}C-NMR spectroscopy for the full B vs. T phase diagram with a critical field of B=14.9T [1]. With an in general very satisfying agreement between experiment and theory, we found a divergence of the low frequency spin dynamics in the critical field regime and a spin gap opening linear with field in the saturated phase. On our poster, we also present NMR studies of the ^{14}N-site in the nitrate groups. Since the ^{14}N-nucleus has a finite quadrupole moment, fluctuations of the electrical field gradient(EFG) tensor become visible in the experiment. By analysis of the angular dependence of the NMR properties it is possible to distinguish between the magnetic and EFG fluctuations for the data presented at temperatures between 2K and 55K and fields B<7T.

[1] H. Kuehne et al., arXiv:0804.2170.

TT 6.68 Mon 13:00 P1A

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

$BaCo_2V_2O_8$ contains screw chains of CoO_6 octahedra which are running along the c axis of the tetragonal crystal structure and are separated by nonmagnetic Ba^{2+} und V^{5+} ions in the aa plane. Due to a compression of the octahedra along c the threefold degeneracy of the t_{2g} orbitals is lifted and the magnetic ground state can be described by an effective Ising spin-1/2 antiferromagnetic chain. In zero magnetic field $BaCo_2V_2O_8$ shows long-range antiferromagnetic order below $T_N \simeq 5.5$ K with the spins oriented along c. The magnetic field influence is highly anisotropic. For magnetic fields applied in the aa plane T_N is only weakly suppressed, e.g. $T_N \simeq 4.5$ K for $H = 8$ T. In case of H parallel c, however, the Néel order is completely sup-

pressed already for fields above about 4 T. Thus, $BaCo_2V_2O_8$ is ideally suited to study this field-induced quantum phase transition. We have prepared single crystals of $BaCo_2V_2O_8$ by a spontaneous nucleation method and have performed measurements of the magnetization, the specific heat, the thermal expansion, and the magnetostriction. These results will be compared to existing theory.
This work is supported by the DFG through SFB 608.

TT 6.69 Mon 13:00 P1A

Anisotropic length changes in $Sr_3Ru_2O_7$ — •Christian Stingl and Philipp Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen

In the itinerant metamagnet $Sr_3Ru_2O_7$, a first order metamagnetic transition is suppressed to a quantum critical end point (QCEP) at $T = 0$ by applying a magnetic field $\mu_0 H_c \approx 8\,\mathrm{T}$ along the c-axis. Quantum critical behaviour is observed in thermal expansion and can be explained in terms of 2d ferromagnetic fluctuations.[1]

Below 1 K, a new phase with a strongly enhanced residual resistivity forms in the vicinity of the QCEP. When H has a small in-plane component, the resistivity becomes anisotropic, which is discussed in terms of formation of a symmetry-broken electronic nematic fluid organized into domains.[2]

Because of the strong magnetoelastic coupling, this reduction of symmetry could also be expected to lead to a distortion of the tetragonal lattice planes. The new phase could therefore be characterized by investigating thermal expansion and magnetostriction in the *ab*-plane perpendicular to the field.

For these measurements, we are testing a new miniaturized capacitive dilatometer, which can be rotated in the field and allows measuring length changes in various orientations relative to field and crystal axes.

This work is in collaboration with F. Weickert, R. Küchler, R.S. Perry and Y. Maeno.

[1] P. Gegenwart et al., PRL **96**, 136402 (2006)
[2] R.A. Borzi et al., Science **315**, 214-217 (2007)

TT 6.70 Mon 13:00 P1A

Quantum Criticality in Ce$M$$In_5$-Systems Studied by Low-Temperature Thermal Expansion — •Jan Guido Donath[1], Philipp Gegenwart[1,3], Eric D. Bauer[2], John L. Sarrao[2], and Frank Steglich[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Los Alamos National Laboratory, Los Alamos, New Mexico, 87545 USA — [3]I. Physikalisches Institut, Universitaet Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany

Ce$M$$In_5$-115-systems are of tremendous current interest since they are ideal to study the interplay of unconventional superconductivity (SC), long-range magnetic order and non-Fermi liquid behavior (nFL).

In this work, we will present low temperature thermal expansion measurements of $CeIrIn_5$, a heavy fermion superconductor at ambient pressure. By applying high magnetic fields $B > 12\,\mathrm{T}$, SC is suppressed and nFL behavior develops, which is believed to be connected to a metamagnetic quantum critical point (QCP) at $B \approx 25\,\mathrm{T}$ [1].

Thermal expansion is a powerful tool to analyse quantum critical behavior and make robust statements about the nature of the QCP. We performed measurements in magnetic fields up to B=17.5 T and temperatures $50\,\mathrm{mK} \leq T \leq 4\,\mathrm{K}$. We will analyse the temperature dependences of our results and compare them with theoretical predictions [2] and other representatives of the 115-family (M=Co, Rh).

[1] Capan *et al.*, PRB **70** 180502 (2004).
[2] Zhu *et al.*, PRL **91** 066404 (2003).

TT 6.71 Mon 13:00 P1A

Low-temperature heat capacity of $Yb(Rh_{0.93}Co_{0.07})_2Si_2$ — •Alexander Steppke, Niels Oeschler, Cornelius Krellner, Manuel Brando, Christoph Geibel, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

Exotic non-Fermi liquid behavior of the Sommerfeld coefficient C/T was reported for the heavy-fermion compound $YbRh_2Si_2$ [1]. It exhibits antiferromagnetic ordering at $T_N = 72$ mK and a quantum critical point (QCP) can be induced by a magnetic field of $\mu_0 H_c = 60$ mT. The application of hydrostatic pressure yields a shift of T_N to higher temperatures and the appearence of a second phase transition at T_L [2].
Instead of using hydrostatic pressure, similar behavior can be achieved by slightly substituting isoelectronic Co on the Rh site without introducing much disorder. At 7% Co substitution T_N is shifted to 400 mK and T_L to 70 mK.
We investigated the specific heat of a $Yb(Rh_{0.93}Co_{0.07})_2Si_2$ high-quality single crystal in magnetic fields and in the temperature range between 0.05 and 4 K. The $T - H$ phase diagram has been explored by means of thermodynamics. The nature of the lower transition and the behaviour of C/T close to the QCP at $\mu_0 H_c \approx 200$ mT has been studied in detail.

[1] J. Custers et al. Nature **424**, 524 (2003).
[2] S. Mederle et al., J. Phys. Condens. Matter **14**, 10731 (2002).

TT 6.72 Mon 13:00 P1A

Pressure tuning of magnetism and superconductivity in $CeCu_2Si_2$ — •Koji Kaneko[1,2], Oliver Stockert[1], Julia Arndt[1], Astrid Schneidewind[3,4], Hirale S. Jeevan[1], Christoph Geibel[1], and Franck Steglich[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]ASRC, Japan Atomic Energy Agency, Ibaraki, Japan — [3]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [4]Neutronenforschungsquelle Heinz-Maier-Leibnitz (FRM-II), TU München, Garching, Germany

In order to get insights on the relationship between magnetism and superconductivity in $CeCu_2Si_2$, neutron scattering experiments under pressure on A-$CeCu_2Si_2$ were carried out. An application of a small pressure of ∼5 kbar for A-$CeCu_2Si_2$ can change the ground state from antiferromagnetic to superconducting through the coexistence phase, which gives the opposite effect to Ge doping. We started from the development of a new pressure cell made of a special aluminum alloy, in order to overcome difficulties of pressure experiments, such as higher background from the cell. This new pressure cell was succeeded to hold the required pressure of more than 3 kbar, which is sufficient to kill antiferromagnetism and enter into the superconducting state. Neutron scattering experiments on PANDA at FRM-II confirm the disappearance of the long-range antiferromagnetic order under pressure, whereas weak magnetic signal still remains at the ordering wave vector. The identical behavior was observed for the S-$CeCu_2Si_2$ with decreasing temperature[1]. Inelastic neutron scattering experiments are currently in progress.

[1] O. Stockert *et al.*, Physica B **403**, 973 (2008).