TT 33: Postersession Correlated Electrons: Metal Insulator Transition, Spin Systems and Itinerant Magnets

Time: Wednesday 14:00–18:00 Location: P1A

TT 33.1 Wed 14:00 P1A

Optical conductivity and correlated bands of $LaVO_3$ and YVO_3 — •David Heilmann and Eva Pavarini — Institut für Festkörperforschung, Forschungzentrum Jülich, 52425 Jülich, Germany

We calculate the optical conductivities and momentum-resolved spectral functions for the $3d^2$ vanadates $LaVO_3$ and YVO_2.

As a method we adopt the LDA+DMFT technique, using Quantum Monte Carlo as an impurity solver. We obtain the self-energy matrix on the real axis by means of the Maximum-Entropy technique and a self-consistent procedure. We use the self-energy matrix to calculate the correlated band structure and the optical conductivity of $LaVO_3$ and YVO_2 both for the high-temperature orthorhombic and the low-temperature monoclinic structure. The effects of orbital fluctuations are discussed.

TT 33.2 Wed 14:00 P1A

Thermodynamic and electrical properties of EuC_{2+x} — •Oliver Heyer[1], Derk Wandner[2], Nils Hollmann[1], Uwe Ruschewitz[2], Thomas Lorenz[1], and John A. Mydosh[1] — [1]II. Physikalisches Institut, Universiät zu Köln, D-50937 Köln — [2]Institut für Anorganische Chemie, Universität zu Köln, D-50939 Köln

We have investigated the magnetization M, specific heat c_p and resistivity ρ of high-purity EuC_{2+x} (-0.1$\leq$ x $\leq$ 0.3) compounds. The magnetization of EuC_2 shows a ferromagnetic ordering at $T_C \simeq 14$K with a saturation moment of $\simeq 7\frac{\mu_B}{FE}$. This imply that EuC_2 is composed of Eu^{2+} and the acetylide ion (C_2^{2-}). T_C hardly changes with x. In the paramagnetic phase all compounds are semiconductors with small bandgaps ($10-20$meV). A very interesting feature is that the onset of the ferromagnetic order decreases the resistivity ρ over several orders of magnitude indicating a metal-insulator transition (MIT). Applying magnetic fields up to 14 tesla, we find a systematic shift of the MIT temperature to higher values, resulting in a colossal magnetoresistance with changes in the resistivity up to 6 orders of magnitude. This behaviour resembles the colossal magnetoresistance of the better known Eu-rich EuO. Furthermore we carried out magnetization and specific heat measurements of YbC_2. The data identify this compound as a diamagnet without structural phase transitions. On this account YbC_2 is used as a non magnetic reference system.

TT 33.3 Wed 14:00 P1A

Co-tunneling in two-dimensional lattices of EBID-nanoparticles — •Roland Sachser, Fabrizio Porrati, and Michael Huth — Physikalisches Institut, Johann Wolfgang Goethe-University, Frankfurt am Main, Germany

W-based granular metals have been prepared by electron beam induced deposition (EBID) from the tungsten-hexacarbonyl-precursor $W(CO)_6$. In EBID the electron beam raster process is reflected in the deposit in the limit of large dwell times. This results in a two-dimensional lattice of mesoscopic granular metal islands, in which metallic nanocrystals are separated by an insulating matrix. The islands have a high tungsten-content and therefore a high intrinsic conductivity. To investigate the transport mechanism we performed transport measurements over a temperature range from 2K to 260K. For low temperatures we observe a $\sigma \sim exp(-(T_0/T)^{1/2})$ dependence of the conductivity. The current-voltage-characteristics do not show a Coulombblockade. We interpret our measurements for low temperatures as a fingerprint of co-tunneling. By changing the electron beam parameters the size of the islands and the lattice constant can be varied. In this way it is possible to adjust the coupling between the islands and influence the transport mechanism.

TT 33.4 Wed 14:00 P1A

Orbital and charge ordering in CuI_2S_4 thiospinel studied by Raman scattering — •Vladimir Gnezdilov[1,2], Peter Lemmens[2], Yurii Pashkevich[3], Kwang-Yong Choi[4], and Vladimir Tsurkan[5] — [1]ILTP, Kharkov, Ukraine — [2]IPKM, TU Braunschweig, Germany — [3]Donetsk Phystech, Ukraine — [4]Chung-Ang Univ., Seoul, Korea — [5]IAP, Chisinau, Moldova

CuI_2S_4 displays a metal-insulator (MI) transition at 230 K with an abrupt decrease of the electrical conductivity and a loss of localized magnetic moments [1]. Below T_{MI} CuI_2S_4 undergoes a simultaneous charge ordering and spin-dimerization transition [2] – a rare phenomenon in three-dimensional compounds. Here we present a Raman scattering study of CuI_2S_4 through the MI transition showing drastic changes of the spectra below T_{MI} consistent with the formation of isotropic Ir^{3+} and Ir^{4+} octamers and spin dimerization [2].

[1] T. Furubayashi et al., J. Phys. Soc. Jpn. 63, 3333 (1994).
[2] P.G. Radaelli et al., Nature 416, 155 (2002).

TT 33.5 Wed 14:00 P1A

The Fermi Surface of MoO_2 as studied by photoelectron spectroscopy, de Haas-van Alphen measurements and electronic structure calculations — •Jörg Kündel[1], Judith Moosburger-Will[1], Siegfried Horn[1], Udo Schwingenschlögl[2], and Volker Eyert[3] — [1]Experimentalphysik II, Universität Augsburg — [2]Theoretische Physik II, Universität Augsburg — [3]Center for Electronic Correlations and Magnetism, Universität Augsburg

A comprehensive study of the electronic properties of monoclinic MoO_2 from both an experimental and a theoretical point of view is presented. We focus on the investigation of the Fermi body and the band structure using angle resolved photoemission spectroscopy, de Haas-van Alphen measurements, and electronic structure calculations. For the latter, the new full-potential augmented spherical wave (ASW) method has been applied. Very good agreement between the experimental and theoretical results is found. In particular, all Fermi surface sheets are correctly identified by all three approaches.

Our results underline the importance of electronic structure calculations for the understanding of MoO_2 and the neighbouring rutile-type early transition-metal dioxides. This includes the low-temperature insulating phases of VO_2 and NbO_2, which have crystal structures very similar to that of molybdenum dioxide and display the well-known prominent metal-insulator transitions.

TT 33.6 Wed 14:00 P1A

Lattice distortions in oxide heterostructures — •Cosima Schuster[1] and Udo Schwingenschlögl[2] — [1]Institut für Physik, Universität Augsburg, D-86135 Augsburg — [2]ICCMP, Universidade de Brasilia, 70904-970 Brasilia-DF, Brazil

Perovskite heterostructures from transition metal oxides have attracted recent interest due to the discovery of metallic interlayers in an otherwise semiconducting system. For example, a metallic contact between two common band insulators is realized in the $LaAlO_3/SrTiO_3$ heterointerface. Nevertheless, it was shown experimentally that the $LaAlO_3$ surface layer must reach a critical thickness of 4 unit cells for the interface to become conducting. This surface effect can be explained by first-principles electronic structure calculations. On varying the thickness of the $LaAlO_3$-layer on a $SrTiO_3$-substrate with a vacuum layer of at least 12 Å thickness, we have found that the interface conduction states are subject to almost rigid band shifts due to a modified Fermi energy. In addition, we take into account structural relaxation at both the $LaAlO_3/SrTiO_3$ interface and the $LaAlO_2$ surface. Drastic alterations are obtained on variation of the layer thicknesses. The distortion of the TiO_6 octahedra in the four layer structure is comparable to the multi-layer system (without surface) and enhances the metallicity in the vicinity of the interface. Modified and enhanced lattice distortions in the two layer system support an insulating state. Cooperative effects induced by the interplay between the interface/surface lattice relaxation and the electrostatic charge depletion explain the matal insulator transition.

TT 33.7 Wed 14:00 P1A

Prediction of insulator to metal transition in rubidium sesquioxide (Rb_4O_6) under high pressure — •S. Shahabeddin Naghavi[1], Gerhard H. Fecher[1], Claudia Felser[1], Jürgen Kübler[2], and Klaus Doll[3] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — [2]Institut für Festkörperphysik, Technische Universität Darmstadt, D-64289 Darmstadt, Germany — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

We report on theoretical predictions of the insulator-metal transition

in rubidium sesquioxide (Rb_4O_6) under high pressure implemented by crystal06 code. Two types of oxygen molecules exist in the sesquioxide Rb_4O_6; these are the paramagnetic hyperoxide O_2^- (two times) and the peroxide O_2^{--} (one molecule). By choosing the ferromagnetic solution and distinguishing between the two different kinds of oxygen molecules, the symmetry is reduced from cubic structure with the symmetry $I\bar{4}3d$ to tetragonal ($I\bar{4}2d$). By increasing the pressure, the differences in the bond-lengths between paramagnetic hyperoxide and peroxide is reduced until finally at a pressure of 162 Gpa they become the same. Moreover, at this pressure, the insulating state becomes metallic and the magnetism disappears. Independent calculations indicate that the equalization of the bond-lengths is essential for loosing the magnetic properties.

TT 33.8 Wed 14:00 P1A

Electronic excitation spectra on undoped and electron doped TiOCl — •Roberto Kraus[1], Martin Knupfer[1], Michael Sing[2], and Ralph Claessen[2] — [1]IFW-Dresden, D-01069 Dresden, Deutschland — [2]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg

TiOCl as a low dimensional Mott insulator and a spin-Peierls compound has reached a lot of interest in the last years. TiOCl is a $3d^1$ system with a half filled band. One way to reach a metal-insulator transition is a filling-controlled method by doping with electrons. In TiOCl exists a large van der Waals gap in the chlorine layers which can be intercalated easily, in our case with potassium. We present the electronic excitation spectrum of TiOCl measured by electron energy loss spectroscopy. For the undoped case we find no dispersion of the excitation above the Mott-gap. With increased doping this excitation splits into a lower and higher lying part. We also investigate the changes of the crystal structure with electron diffraction and find a complex behavior with different superstructures and an expanding lattice constant perpendicular to the Ti chains.

TT 33.9 Wed 14:00 P1A

Doping dependence of stripe order in $La_{2-x}Sr_xNiO_{4+\delta}$ — •Christoph Trabant[1], Hsueh-Hung Wu[1,2], Marcel Buchholz[1], Enrico Schierle[3], Mohammed Benomar[1], Agung Nugroho[4], Alexander Komarek[1], Ralf Feyerherm[3], Markus Braden[1], Liu Hao Tjeng[1], and Christian Schüssler-Langeheine[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]NSRRC, Hsinchu, Taiwan — [3]Helmholtz-Zentrum Berlin — [4]Bandun University, Indonesia

Stripe order in $La_{2-x}Sr_xNiO_{4+\delta}$ with a doping level $n_h = x + 2\delta$ between 0.2 and 0.33 exhibits an unusual temperature dependence of the correlation length, which goes through a maximum at intermediate temperatures and decreases not only upon heating but also upon cooling. While the integrated intensity of the charge and spin order peak is conserved, the system breaks into smaller and smaller domains when cooled.

We studied this behavior as a function of Sr and oxygen content using resonant diffraction at the Ni $2p \rightarrow 3d$ ($L_{2,3}$) and $1s \rightarrow 4p$ (K) thresholds. The goal is to understand the mechanism for the low-temperature broadening. Differences between commensurate and incommensurate order as well as the effect of the oxygen content will be discussed.

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TT 33.10 Wed 14:00 P1A

The coupled electronic order of manganese and oxygen states in doped manganites — •Jochen Geck[1,2], David G. Hawthorn[3], Kyle M. Shen[4], Hiroki Wadati[2], Enrico Schierle[5], Liu H. Tjeng[6], Hsueh-Hung Wu[6], Christian Schüssler-Langeheine[6], and George A. Sawatzky[2] — [1]IFW Dresden, Germany — [2]University of British Columbia, Canada — [3]University of Waterloo, Canada — [4]Cornell University, USA — [5]Helmholtz-Zentrum Berlin, Germany — [6]University of Cologne, Germany

Comparing resonant soft x-ray scattering (RSXS) experiments and realistic many-body calculations, the nature of the electronic crystal formed in the low-temperature phase of $La_{7/8}Sr_{1/8}MnO_3$ is investigated. The analysis of the experimental data implies that the modulation of the Mn-valence must be very small and that the detected Mn-ordering is mainly of orbital nature. The emerging picture of manganese orbital order, which is coupled to charge and orbital order of the O 2p-states, seems to be a general feature of electronically ordered manganites.

TT 33.11 Wed 14:00 P1A

Investigation of Orbital-Ordering in Sr_2VO_4 — •Joseph M. Law[1,2], Eva Brücher[1], Sukanta Karmakar[1], Karl Syassen[1], and Reinhard K. Kremer[1] — [1]Max Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]Dep. of Physics, Loughborough University, Loughborough, U.K.

Sr_2VO_4 is a Mott insulator which crystallizes with the tetragonal K_2NiF_4 structure. It hosts V^{4+}, ($3d^1$ configuration), is another layered S=1/2 afm with unusual ground state properties. Recently it was shown that tetragonal Sr_2VO_4 undergoes a phase transition (PT) near 104K evidenced by a sudden drop of the magnetic susceptibility and anomalies in the lattice parameters (c increases by 0.15%) but no change of the crystallographic symmetry. Based on *ab initio* calculations the PT was ascribed to an orbital-ordering transition which leads to a decreasing occupancy of the d_{xy} orbital balanced by an increasing electronic density along the c axis.[1] We have investigated the orbital-ordering PT by heat capacity, dc resistivity and dielectric measurements on polycrystalline samples of tetragonal Sr_2VO_4. The heat capacity measurements display an anomaly confirming a PT at 104 K. Additionally, a sluggish precursor regime extending up to 125K consistent with the lattice properties was found. Our resistivity and dielectric measurements prove a Mott gap of $\sim$ 100 meV as already seen in thin films, which reveals an increase of the activation energy below $\sim$ 125 K leading to a rapid growth of the electrical resistance below the PT.

[1] H. D. Zhou *et al.*, Phys. Rev. Lett. **99**, 136403 (2007).

TT 33.12 Wed 14:00 P1A

Interplay between superconductivity and charge order in 2D organic superconductors — •Stefan Kaiser[1], Natalia Drichko[1], Yaxiu Sun[1], Martin Dressel[1], Toomas Room[2], Dan Hüvonen[2], Urmas Nagel[2], Matteo Masino[3], Alberto Girlando[3], and John Schlueter[4] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]KBFI, Tallinn, Estonia — [3]Dip. Chimica G.I.F. and INSTM-UdR Parma, Italy — [4]Material Science Division, Argonne National Laboratory, U.S.A.

Theoretical study of systems with quarter-filled conductance band and strong electron-electron correlations propose superconductivity mediated by charge order fluctuations [1]. We present IR reflectivity of a 1/4-filled organic superconductor β"-(BEDT-TTF)2SF5CH2CF2SO3 (Tc=5 K) in the frequency range between 8 and 10000 cm-1 at temperatures down to 1.8 K. Our spectroscopic study reveals a splitting of the charge-sensitive phonons showing charge order while transport properties show metallic behavior. The narrow Drude response and its interplay with charge fluctuations, evident in an electronic band, is responsible for superconductivity, with a superconducting gap of 12 cm-1 at 1.8 K. A comparison with the isostructural metal β"-(BEDT-TTF)2SF5CHFSO3 reflects the close relation between superconductivity and charge order.

[1]. J. Merino et al. Phys. Rev. Lett 87, 237002 (2001)

TT 33.13 Wed 14:00 P1A

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

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

TT 33.14 Wed 14:00 P1A

A Functional Approach for the Spin Chain — •Stephan Filor and Thomas Pruschke — Institut für Theoretische Physik, Universität Göttingen

We set up a new approach to the physics of spin systems which uses

a resolvent method originally proposed by Keiter and Kuramoto. In analogy to the Baym-Kadanoff formalism the latter introduced the partition sum of a system as a functional of the resolvent of the Hamiltonian and its so called generalized self-energy. This functional is the starting point for a variational cluster method which is based on Potthoffs self-energy functional approach. In a first step we apply our ansatz to a Heisenberg spin chain.

TT 33.15 Wed 14:00 P1A

Spin-1 anisotropic Heisenberg antiferromagnets — •David Peters[1], Ian McCulloch[2], and Walter Selke[1] — [1]RWTH Aachen University and JARA-SIM, Germany — [2]The University of Queensland, Australia

Intricate phase diagrams of spin-1 Heisenberg antiferromagnets with exchange and single-ion anisotropy are studied using mainly density matrix renormalization group techniques.

Various phases are identified, including antiferromagnetic, spin-liquid (or spin-flop), supersolid (or biconical), and ferromagnetic phases. Results are compared to recent findings on related quantum models and to properties of corresponding classical spin systems.

Funded by the Excellence Initiative of the German federal and state governments.

TT 33.16 Wed 14:00 P1A

Spin-Dynamics of the antiferromagnetic S=1/2-Chain at finite magnetic Fields and intermediate Temperatures — •Simon Grossjohann and Wolfram Brenig — Institut für theoretische Physik, Technische Universität Braunschweig

We present results for the dynamic structure factor of the antiferromagnetic spin-1/2 Heisenberg chain at finite temperatures and finite magnetic fields. Using Quantum-Monte-Carlo based on the stochastic series expansion and Maximum-Entropy methods we detail the evaluation of longitudinal and transverse dynamic structure factors $S^{\alpha\beta}(q,\omega)$ with $\alpha\beta \in \{zz, xx, +-, -+\}$ from vanishing magnetic fields up to and above the threshold B_c for ferromagnetic saturation, as well as for high and for intermediate temperatures. The field-induced redistribution of spectral weight was focus of our studies, contrasting longitudinal versus transverse excitations. At finite fields below saturation incommensurate low-energy modes are found to be consistent with zero temperature Bethe-Ansatz. The crossover between the field induced ferromagnet above B_c and the Luttinger liquid below B_c is analyzed in terms of the transverse spin-dynamics and compared to T_1-relaxation rates on CuPzN. Finally we assess the quality of the analytic continuations by evaluating sum-rules and detailed balance to demonstrate excellent consistency of the Maximum-Entropy results.

TT 33.17 Wed 14:00 P1A

Magnetic impurities in two-dimensional spin-1/2 antiferromagnets — •Björn Willenberg, Simon Grossjohann, and Wolfram Brenig — Institut für theoretische Physik, Technische Universität Braunschweig

Using Quantum Monte-Carlo methods based on the stochastic series expansion we investigate a single spin degree of freedom coupled to a two-dimensional Heisenberg antiferromagnet (HAFM). Results will be presented for thermodynamic and dynamic properties. In particular the local susceptibility will be considered as a function of temperature, magnetic field, and local spin quantum number. Moreover we will contrast the case of antiferro- versus ferromagnetic coupling of the impurity to the HAFM. This analysis will be extended to real-space spin correlation-functions which will be evaluated in the vicinity of the quantum impurity including a detailed finite size analysis. Finally the impurity dynamics will be considered by calculating imaginary time spin-correlators and performing Maximum Entropy analysis.

TT 33.18 Wed 14:00 P1A

Effective Hamiltonians for Doped Spin-$\frac{1}{2}$ Ladders from Self-Similar Continuous Unitary Transformations — •Sebastian Duffe, Tim Fischer, and Götz S. Uhrig — Technische Universität Dortmund

Doped spin-$\frac{1}{2}$ ladder systems are important model systems for 2D high-T_C superconductors. Their one-dimensionality renders them more tractable to various analytic and numerical approaches. Experimentally such ladder systems are realized in the so-called telephone number compounds $Sr, Ca, La_{14}Cu_{24}O_{41}$.
Here we systematically derive effective Hamiltonians for the hole motion in such spin ladders. The technique of choice are continuous unitary transformations (CUTs) which are performed self-similarly for the coefficients of operator monomials in real space in second quantization. The proliferating number of terms is bounded by truncating far reaching processes which reach longer than the finite correlation length. The magnetic excitations are triplons on the rungs of the ladder; the charge excitations are holes with spin living also on the rungs of the ladder. The effective Hamiltonian allows us to read off the dispersions of single excitations directly. But it also contains their interaction.

TT 33.19 Wed 14:00 P1A

Thermodynamics of a one-dimensional frustrated spin-$\frac{1}{2}$ Heisenberg ferromagnet — •Moritz Härtel[1], Johannes Richter[1], Dieter Ihle[2], and Stefan-Ludwig Drechsler[3] — [1]ITP, OvG-Universität Magdeburg, D-39016 Magdeburg, Germany — [2]ITP, Universität Leipzig — [3]Leibniz-Institut IFW Dresden

The frustrated one-dimensional J_1-J_2 Heisenberg ferromagnet ($J_1 = -1$, $J_2 > 0$) has attracted much attention due to recent experiments on edge-shared chain-cuprates, e.g. $LiVCuO_4$ and Li_2CuO_2.
We use a second-order Green's function technique and the full exact diagonalization of finite systems of up to $N = 22$ lattice sites to calculate thermodynamic properties (correlations functions $\langle \mathbf{S}_0 \mathbf{S}_n \rangle$, correlation length ξ, isothermal spin susceptibility χ, and specific heat C_V). Although we restrict on the ferromagnetic ground state, i.e. $J_2 < 0.25$, the frustration influences the thermodynamics substantially. We find that the critical indeces of the susceptibility and the correlation length are not changed by a finite frustration in absence of a magnetic field, i.e. $\chi = y_0 T^{-2}$ and $\xi = x_0 T^{-1}$ at $T \to 0$. The coefficients y_0 and x_0 decrease linearly with increasing J_2 and vanish at the critical point $J_2 = 0.25$ due to the zero-temperature phase transition that is accompanied by a change in the critical behavior. In addition, we detect the existence of an additional low-temperature maximum in the specific heat when approaching the critical point. Including a weak magnetic field ($h \lesssim 0.07$) this additional maximum exists already at $J_2 = 0$ but gets more pronounced with increasing J_2.

TT 33.20 Wed 14:00 P1A

Thermodynamic properties of the ferromagnetic Kondo Lattice Model at finite temperatures for different magnetic phases — •Martin Stier and Wolfgang Nolting — Humboldt-Universität zu Berlin, Institut für Physik, Theoretische Festkörperphysik, Newtonstraße 15, 12489 Berlin, Germany

We investigate the ferromagnetic Kondo Lattice Model (KLM) at finite temperatures for different (anti)ferromagnetic phases. To compare the theory with real materials like the manganites we extend the pure KLM by terms describing the Coulomb interaction, the superexchange and a Jahn-Teller splitting. Using a modified RKKY method we determine the various transition temperatures and decide by calculating the free energy which phase is actually present at a given parameter set. Additionally, we can evaluate other important thermodynamic quantities like the entropy or the specific heat.

TT 33.21 Wed 14:00 P1A

The ground state phase diagram of the ferromagnetic Kondo-lattice model — •Sören Henning and Wolfgang Nolting — Humboldt Universität zu Berlin; Institut für Physik; AG Festkörpertheorie; Newtonstr.15; 12489 Berlin

The magnetic ground state phase diagram of the ferromagnetic Kondo-lattice model is constructed by calculating internal energies of all possible bipartite magnetic configurations of the simple cubic lattice explicitly. This is done in one dimension (1D), 2D and 3D assuming a local moment of $S = \frac{3}{2}$ and a saturated sub-lattice magnetization. As will be shown, it is possible to treat all higher local correlation functions appearing in the many-body problem exactly under these assumptions. A simple explanation for the obtained phase diagram in terms of bandwidth reduction is given. Regions of phase separation are determined from the internal energy curves by an explicit Maxwell construction.

TT 33.22 Wed 14:00 P1A

Spin waves in the Heisenberg and in the Kondo-lattice Model — •Andrej Schwabe and Wolfgang Nolting — Institut für Physik, Humboldt-Universität, Newtonstraße 15, 12489 Berlin, Germany

We present a new approach to the 3D ferromagnetic Heisenberg model being bosonized by the Dyson-Maleev transformation. Magnon excitation energies and line widths are derived by applying the method of moments with a broadened magnon spectral density.

Furthermore, we extend the investigation to the ferromagnetic Kondo-lattice model that can be mapped onto an effective Heisenberg model by using the modified RKKY interaction and the Interpolating Selfenergy Approach. Magnon energies and line widths are calculated for the limiting cases relevant to manganites and ferromagnetic semiconductors. The dependence on band occupation n, intra-atomic exchange J and temperature is investigated. Both zone boundary magnon softening and anomalous magnon damping are found.

TT 33.23 Wed 14:00 P1A

Manipulating magnetic structures in chiral metals by currents — •Karin Everschor[1], Achim Rosch[1], and Rembert Duine[2] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Institute for Theoretical Physics, Department of Physics and Astronomy Faculteit Betawetenschappen, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

We investigate how currents can modify magnetic structures in bulk materials. In magnets without inversion symmetry, weak spin-orbit coupling leads to the formation of magnetic helices with a long pitch. These helices pin only very weakly to disorder and the underlying crystalline lattice. We start from the Landau-Lifshitz-Gilbert equation including adiabatic and non-adiabatic spin transfer torques. We investigate a variational approach to determine equations of motion for different magnetic structures. Especially interesting is the influence of currents on the so-called "A-phase" of MnSi, where a lattice of skyrmions forms.

TT 33.24 Wed 14:00 P1A

Spectral weight of Mott-Hubbard excitations in YVO_3 studied by ellipsometry — •Julia Küppersbusch[1], Christina Hilgers[1], Agung Nugroho[2], Thomas Palstra[2], and Markus Grüninger[1] — [1]Universität zu Köln — [2]Rijksuniversiteit Groningen

We investigate the optical conductivity of YVO_3 between 0.75 and 5.5 eV from T=15 to 300 K by means of ellipsometry. Different groups reported contradictory data sets, none of them succeeded in explaining the T dependence of the peak structure [1-3].
The compound YVO_3 undergoes a series of temperature-induced structural/electronic phase transitions. The different phases show different spin/orbital ordering patterns, leading to a pronounced anisotropy in the optical spectra. The Mott-Hubbard gap of insulating YVO_3 is located at 1.6 eV. The strong increase of the optical conductivity above 4 eV is attributed to the onset of charge-transfer (CT) excitations. Below the CT transitions, the optical spectrum shows a three-peak structure with a complex T dependence. This has been attributed to the different types of spin/orbital ordering, but a consistent description could not be achieved. Our data resolve the issue of the contradictory data sets. We discuss the multiplet assignment of the different peaks and obtain an excellent understanding of the T dependence of the optical conductivity.

[1] S. Miyasaka, Y. Okimoto, and Y. Tokura, J. Phys. Soc. Jpn. **71**, 2086 (2002).
[2] A.A. Tsvetkov *et al.*, Phys. Rev. B **69**, 075110 (2004).
[3] J. Fujioka, S. Miyasaka, and Y. Tokura, PRB **77**, 144402 (2008).

TT 33.25 Wed 14:00 P1A

Synthesis and properties of the filled skutterudites $CePt_4Ge_{12}$ and $SmPt_4Ge_{12}$ — •Walter Schnelle, Roman Gumeniuk, Andreas Leithe-Jasper, Helge Rosner, Michael Nicklas, Michael Baenitz, Michael Schöneich, Marcus Schmidt, Ulrich Schwarz, and Yuri Grin — MPI für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden, Germany

While the ternary platinum-germanium skutterudites with the trivalent rare-earths La and Pr are superconductors the isostructural compounds with Ce, Nd^{3+} and Eu^{2+} order antiferromagnetically [1]. Recently, isotypic $SmPt_4Ge_{12}$ was prepared at high pressure and XAS measurements reveal that the valence of samarium is temperature-independent and close to 3+. Magnetization data show typical van-Vleck paramagnetic behaviour at elevated temperatures. The low-temperature specific heat displays a field-independent Schottky-type anomaly and a large linear coefficient γ. CePt4Ge$_{12}$ shows a typical valence fluctuation behaviour with an average Ce valence close to 3+. Together with electronic band structure calulations and NMR investigations [2] we discuss the low-temperature behaviour of these new compounds.

[1] R. Gumeniuk *et al.* Phys. Rev. Lett. 100 (2008) 017002.
[2] M. Baenitz *et al.* this conference.

TT 33.26 Wed 14:00 P1A

Spin-phonon scattering and heat transport in spin ladders — •Christina Seidler and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

We study the spin-phonon dynamics and the heat transport of two-leg spin-1/2 ladders in the presence of a magnetoelastic deformation-potential coupling. In the limit of weak inter-rung exchange we employ a mapping of the spin degrees of freedom to a gas of non-interacting bond-bosons to describe the magnetic excitations. The coupled spin-phonon excitations are derived perturbatively and their spectra will be discussed as a function of momentum, frequency, temperature, system parameters and external magnetic fields. Both optical and acoustical phonons will be considered.

The heat transport will be investigated in the linear-response regime by evaluating the corresponding Kubo integrals. Results for the temperature and the magnetic field dependence of both, the magnetic and phononic heat conductance, will be presented. In particular the effect of the field-induced triplet softening will be regarded.

Our results will be put into the context of the anomalous magnetic heat transport of the spin-ladder compound $Sr_{14}Cu_{24}O_{41}$.