TT 14: Spin Systems and Itinerant Magnets

Time: Tuesday 14:00–19:15 Location: H19

TT 14.1 Tue 14:00 H19

Static and Dynamic Properties of an [Fe_{13}] Cluster — •Joris van Slageren[1], Patrick Rosa[2], and Andrea Caneschi[3] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]ICMCB, CNRS, Pessac, France — [3]INSTM, UdR Firenze, University of Florence, Italy

The static and dynamic magnetic properties of an [Fe_{13}] cluster were investigated using several experimental techniques. The cluster crystallizes in a cubic space group, but careful investigation of the crystallographic data revealed that the symmetry is distorted locally. DC magnetic susceptibility measurements showed the presence of competing antiferromagnetic isotropic exchange interactions leading to a high-spin ground state and many low-lying excited spin states, which was confirmed by inelastic neutron scattering measurements. From high-field electron paramagnetic resonance measurements a small zero-field splitting of the spin ground state was inferred, which supports the local symmetry distortion found in the crystallographic studies. The spin dynamics slows down at sub-kelvin temperatures, where ac susceptibility measurements indicated that part of the sample shows superparamagnetic-like behavior and the other part relaxes through magnetization tunneling. The Mössbauer data confirmed the slowing down of the spin dynamics, indicating that this occurs mainly in the peripheral spins.

TT 14.2 Tue 14:15 H19

Hall effect and magnetoresistance in weakly ferromagnetic $CeSi_x$ and heli-magnetic MnSi — Andreas Neubauer[1], Christian Pfleiderer[1], Philipp Niklowitz[1], Robert Ritz[1], •Peter Böni[1], Dmitri Souptel[2], and Günter Behr[2] — [1]Physik Department E21, Technische Universität München, D-85748 Garching, Germany — [2]IFW Dresden, PF 270116, D-01171, Dresden, Germany

We report a comparison of the magnetoresistance and Hall effect in single crystals of the easy-plane ferromagnet $CeSi_x$ ($x \approx 1.81$) with that observed in the helical magnet MnSi. In $CeSi_x$ the anomalous Hall effect clearly tracks the ordered moment as function of temperature and magnetic field. It may be used as a simple means to establish the presence of a ferromagnetic quantum phase transition under pressure. The behavior seen in ferromagnets $CeSi_x$ is contrasted by anomalous contributions to the Hall effect in MnSi, which suggest an important scale of order 100K. Further, in MnSi only subtle differences in the temperature dependences of the Hall effect near a quantum phase transition may be expected. We compare a conventional analysis in the framework of additive charge carrier relaxation rates with the more recent proposal of additive currents.

TT 14.3 Tue 14:30 H19

Magnetic excitations in multiferroic $TbMnO_3$ — •Daniel Senff[1], Peter Link[2], Klaudia Hradil[3], Arno Hiess[4], Louis Pierre Regnault[4], Yvan Sidis[5], Nadir Aliouane[6], Dimitri Argyriou[6], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Forschungsneutronenquelle FRM II, TU München — [3]Institut für Physikalische Chemie, Universität Göttingen — [4]Institut Laue-Langevin, Grenoble / France — [5]Laboratoire Leon Brillouin, Saclay / France — [6]Hahn-Meitner-Institut, Berlin

Ferroelectricity (FE) in $TbMnO_3$ is intimately coupled to a complex magnetic ordering: The existence of a spontaneous electric polarization is closely correlated with a magnetic transition into an incommensurable spin-spiral structure. The critical excitations at the FE-transition are thus no longer of phononic, as in conventional ferroelectrics, but of magnetic origin.

We present extensive neutron scattering studies on the spin-wave spectrum of $TbMnO_3$ in the para- as well as in the ferroelectric phase [1]. We have identified the different magnon branches of the spiral structure and discus the dispersion, the field and the temperature dependence of the modes most relevant for the FE-transition. Comparing with recent optical experiments we find an excellent agreement and strengthen the interpretation of strongly mixed magnon-phonon excitations, called electromagnons, as proposed by Pimenov et al. [2].

[1] D. Senff et al., cond-mat/0610620, submitted to PRL.
[2] A. Pimenov et al., Nature physics **2** (2005) 97.

TT 14.4 Tue 14:45 H19

Modelluntersuchungen zum Phasendiagramm multiferroischer Manganite — •Jens Wohlgemuth und Gertrud Zwicknagl — Institut für Mathematische Physik, Technische Universität Braunschweig, Braunschweig

Es werden die Grundzustände eines Modell-Hamilton-Operators zur Beschreibung von $R\mathrm{MnO_3}$ (R=Tb, Dy, Gd) diskutiert. Als Modell wird das zweifachentartete Doppel-Austausch-Modell mit antiferromagnetischer Kopplung zwischen benachbarten t_{2g} Spins verwendet. Dieses wird um die Dzyaloshinskii-Moriya-Wechselwirkung erweitert, die durch das Brechen der Inversionssymmetrie eine makroskopische elektrische Polarisation erzeugen kann. Die mögliche Grundzustände werden zunächst in Molekularfeldnäherung bestimmt. Dabei wird die kinetische der e_g-Bandelektronen exakt behandelt. Das Auftreten von Phasenseparation wird untersucht. Schließlich werden Quantenkorrekturen zur klassischen Rechnung diskutiert.

Invited Talk TT 14.5 Tue 15:00 H19

Topological phases in condensed matter — •Roderich Moessner — Theoretical Physics, Oxford University

Topological phases currently play an important role in condensed matter physics. Most saliently, they are associated with various spectacular phenomena, such as the fractional quantum Hall effect or, with less confidence, high-temperature superconductivity. In addition, they are central to the attempt to construct a quantum computer protected against decoherence by a topological mechanism. Finally, they widen our understanding of the possible states of matter, as their description lies beyond the classial Landau-Ginzburg–Wilson framework of phases and phase transitions. This talk provides an overview of some of these issues, together with a presentation of recent developments. It focuses on the role that magnetic lattice systems can play in elucidating the physics of topological phases.

15 min. break

TT 14.6 Tue 15:45 H19

Static Holes in the Geometrically Frustrated Bow-Tie Ladder — •Wolfram Brenig[1] and George Martins[2] — [1]Institut für Theoretische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [2]Department of Physics, Oakland University, Rochester, MI 48309, U.S.A.

Doping of the geometrically frustrated bow-tie spin ladder with static holes is investigated by a complementary approach using exact diagonalization and hard-core quantum dimers. Results for the thermodynamics in the undoped case, the singlet density of states, the two-hole energy and the spin correlations will be presented. We find that the static holes polarize their vicinity by a localization of singlets in order to reduce the frustration. As a consequence the singlet polarization cloud induces short range repulsive forces between holes with oscillatory longer range behavior, which may lead to deconfinement. For those systems we have studied, most results for the quantum dimer approach agree qualitatively if not quantitatively with exact diagonalization. The ground state of the undoped system is non-degenerate with translationally invariant nearest-neighbor spin correlations up to the largest systems studied, consistent with a spin liquid state or a valence bond crystal with very large unit cell.

TT 14.7 Tue 16:00 H19

Strongly correlated fermions on frustrated lattices — •Frank Pollmann[1], Kirill Shtengel[2], Peter Fulde[1], and Erich Runge[3] — [1]Max–Planck–Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Department of Physics, University of California, Riverside, CA 92521, USA — [3]Technische Universität Ilmenau, Institut für Physik, 98684 Ilmenau, Germany

Systems with frustrated interactions are generally characterized by a high density of low–lying excitations which leads to a high susceptibility and thus interesting physical effects. The study of frustrated spin systems has revealed numerous fascinating properties, e.g., the realization of liquid phases and an enhanced magnecaloric effect. We focus on charge degrees of freedom on geometrically frustrated lattices. In particular, we study a novel class of strongly correlated fermions which could allow for a possibility of fractionally charged excitations. For a model of strongly correlated spinless fermions on a planar pyrochlore

(checkerboard) lattice it has been shown that fractional charges are linearly confined. We consider now a model of spinful fermions on a geometrically frustrated kagome lattice at particular filling factors. Of special interest is again the strongly correlated limit where excitations which carry a fractional charge are possible. An effective Hamiltonian is derived which describes the low–lying excitations. We study the interplay between charge– and spin–degrees of freedom by means of exact diagonalization. In particular we show that the ground state is charge and spin ordered.

TT 14.8 Tue 16:15 H19

Correlated spinless fermions on a checkerboard lattice — •Olga Sikora, Frank Pollmann, and Peter Fulde — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

Possible fractionalization of quantum numbers on frustrated lattices has recently attracted a lot of interest. In particular, it has been suggested that charge fractionalization might occur in a model of strongly correlated spinless fermions on a planar pyrochlore (checkerboard) lattice.

We consider a quarter– and half–filled checkerboard lattice in the limit of strong nearest–neighbor interactions V ($V \gg |t|$, where t is a hopping integral). The low–energy excitations are described by an effective Hamiltonian which is given to the lowest non-vanishing order by ring exchange around hexagons. A gauge transformation allows to remove the fermionic sign problem and the system can be described by an effective bosonic model. We use the Green's function Monte Carlo method to study the quantum mechanical ground state of the effective Hamiltonian. The method is verified by a comparison with the results for small clusters obtained by exact diagonalization method.

TT 14.9 Tue 16:30 H19

Resonant Inelastic X-ray Scattering at the O 1s Resonance of Transition Metal Monoxides — •Thorsten Schmitt[1], Laurent Duda[2], Vladimir Strocov[1], Martin Magnuson[2], Johan Forsberg[2], Anders Olsson[2], Joseph Nordgren[2], Kozo Okada[3], and Akio Kotani[4] — [1]Swiss Light Source, Paul Scherrer Institut, Villigen PSI, Switzerland — [2]Department of Physics, Uppsala University, Uppsala, Sweden — [3]The Graduate School of Natural Science and Technology, Okayama University, Okayama, Japan — [4]RIKEN/Spring8, Hyogo, Japan

Resonant inelastic x-ray scattering (RIXS) is a powerful tool for determining the energy and symmetry of charge neutral electronic excitations in strongly correlated materials. We report on high-resolution polarization-dependent RIXS at the O 1s resonance of NiO [1], CoO and MnO. The experimental results are compared to multi-site cluster calculations, which are able to describe collective excitations. Tuning the incident X-ray energy to the first absorption peak excites the O 1s electron into empty O 2p states strongly hybridized with the metal 3d states. Thus the de-excitation process reveals contributions from low-energy excitations mediated by the O 1s core-hole. Apart from local oxygen ligand to metal charge transfer excitations and local crystal field excitations, the O 1s RIXS spectra give also rise to non-local metal-to-metal charge transfer excitations and double inter-site spin flip excitations (double-singlet creation).

[1] L.-C. Duda, T. Schmitt, M. Magnuson et al., Phys. Rev. Lett. 96, 067402 (2006).

TT 14.10 Tue 16:45 H19

Study of magnetic ordering in $YTi0_3$ using high-resolution dilatometry — •William Knafo[1,2], Christoph Meingast[1], Alexander Boris[3], Paul Popovich[3], Natalia Kovaleva[3], Petar Yordanov[3], Andrei Maljuk[3], Bernhard Keimer[3], and Hilbert v. Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe — [2]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe — [3]Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart

The perovskite $YTi0_3$ orders ferromagnetically below $T_C = 26.7$ K, whereas $LaTiO_3$ orders antiferromagnetically below $T_N = 150$ K. The origin of this difference is currently being strongly debated and is related to the different types of lattice distortions, e.g. to the $GdFe0_3$-type distortion and to the Jahn-Teller distortion induced by the orbital ordering in these systems [1-5]. We present here a study of the macroscopic distortions associated with magnetic ordering in $YTi0_3$ using thermal expansion and magnetostriction measurements. The uniaxial pressure dependencies of the Curie temperature T_C and of the low temperature ferromagnetic moment are extracted from our data. The coupling of magnetism to the different kinds of distortion (i.e. of $GdFe0_3$- and Jahn-Teller-type) will be discussed.

[1] Ulrich et al., Phys. Rev. Lett. 89, 167202, (2002).
[2] Iga et al., Phys. Rev. Lett. 92, 176403, (2004).
[3] Akimitsu et al., J. Phys. Soc. Jpn. 70, 3475 (2001).
[4] Pavarini et al., New J. Phys. 7, 188 (2005).
[5] Mochizuki and Imada, New J. Phys. 6, 154 (2004).

TT 14.11 Tue 17:00 H19

Ordering and spin waves in vanadium spinels — •Natalia Perkins[1] and Olga Sikora[2] — [1]Technische University of Braunschweig, Braunschweig, Mendellsohnstrasse 3,38106, Germany — [2]Max Planck Institute for Complex System, Noethnitzer Str.38, Dresden, 01187, Germany

We consider the effect of quantum spin fluctuation on the ground state properties of spin-orbital Hamiltonian on a pyrochlore lattice, which is derived to model the ground state properties of vanadium spinel oxides AV_2O_4 (A=Zn, Mg, Cd). As the magnitude of the spin-orbit interaction and that of the exchange one are very similar, both interactions should be simultaneously considered. We show that the low-energy effective Hamiltonian decides about the magnetic interactions of the system and determines the ground state. We also find that the magnetic excitation spectrum obtained by linear spin-wave approach in case of quenched orbital angular momentum differs significantly from one calculated in the magnetic exciton model formulated for the case with unquenched orbital angular momentum. Thus we suggest that the performance of the neutron scattering experiment would help to clarify both the overall picture of the ground state and of the excitation spectrum.

TT 14.12 Tue 17:15 H19

Magnetic properties of the layered cobaltates $La_{2-x}Sr_xCoO_4$ — •N. Hollmann, M.W. Haverkort, M. Benomar, M. Reuther, T. Lorenz, and J.A. Mydosh — II. Physikalisches Institut, University of Cologne

This talk presents a study on the magnetic properties of the layered perovskite $La_{2-x}Sr_xCoO_4$. This class of materials crystallises in the K_2NiF_4 structure as the high-T_C superconductors $La_{2-x}Sr_xCuO_4$ or the corresponding nickelates $La_{2-x}Sr_xNiO_4$, the latter exhibiting stripe order of both charge and spin. In many cobaltates, the spin state of the cobalt ions is an extra degree of freedom. The non-layered compound $LaCoO_3$ even shows a thermally driven spin-state transition. Much less is known about the spin states of the cobalt ions in $La_{2-x}Sr_xCoO_4$. We prepared a series of single crystals by the floating zone method, covering a strontium doping range of $0.3 \leq x \leq 0.8$. We measured the magnetic susceptibility for a magnetic field applied parallel and perpendicular to the CoO_2 planes. We find a clear deviation from Curie-Weiss behaviour and strong anisotropy. From the direction of the magnetic anisotropy we conclude that χ is dominated by Co^{2+} in the high-spin state, while Co^{3+} is in the low-spin state. These findings are confirmed by full-multiplet crystal field calculations which show that spin-orbit coupling and crystal field effects are essential for describing the magnetic behaviour.

Supported by the DFG through SFB 608

15 min. break

TT 14.13 Tue 17:45 H19

Orbitally Ordered Phase in $Ca_{2-x}Sr_xRuO_4$ Investigated with Resonant X-ray Diffraction — •Ioannis Zegkinoglou[1], Joerg Strempfer[2], Britta Bohnenbuck[1], Christie S. Nelson[3], John P. Hill[3], Jonathan C. Lang[4], George Srajer[4], Yoshiteru Maeno[5], and Bernhard Keimer[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]HASYLAB at DESY, Hamburg, Germany — [3]Brookhaven National Laboratory, New York, USA — [4]APS at Argonne National Laboratory, Argonne, USA — [5]Department of Physics, Kyoto University, Japan

Resonant x-ray diffraction at the Ru L_{II} and L_{III} absorption edges was used to investigate the interplay between the spin, lattice and orbital degrees of freedom in the layered 4d-electron $Ca_{2-x}Sr_xRuO_4$ system [1]. A new orbital ordering phase transition was discovered in single-crystal compounds with Sr-doping x=0 and x=0.1 at temperatures 260 K and 130 K, respectively, at reciprocal space positions (100) and (011). The orbital order is only weakly coupled to the lattice. Its propagation vector is not affected by the change of the low-temperature antiferromagnetic structure upon Sr substitution. The tilt order of the

RuO_6 octahedra was also probed in our studies. It produces resonant scattering at the structurally and magnetically forbidden (110) position and follows a different temperature dependence from orbital order.

[1] I. Zegkinoglou et al., Phys. Rev. Lett. 95, 136401 (2005)

TT 14.14 Tue 18:00 H19

Magnetism in single-layered Ruthenates — •Paul Steffens[1], Olaf Schumann[1], Yvan Sidis[2], Peter Link[3], Satoru Nakatsuji[4], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität Köln, 50937 Köln — [2]Laboratoire Léon Brillouin, Gif-sur-Yvette, France — [3]FRM II, Technische Universität München, 85747 Garching — [4]Institute of Solid State Physics, Tokyo, Japan

We present recent results on the magnetism in the single-layered ruthenates $Ca_{2-x}Sr_xRuO_4$. Depending on the Sr-content x, very different properties are observed. In this contribution we focus on the region $0.2 < x < 0.5$. Here, the system is metallic and paramagnetic, but close to magnetic order, and a competition of a ferromagnetic and incommensurate antiferromagnetic instability determines the magnetic behaviour. An applied magnetic field induces a drastic change; we have studied this metamagnetic transition by inelastic neutron scattering, thereby probing the dynamic magnetic correlations at different magnetic fields and temperatures. We find that the ground state without magnetic field is determined by a near nesting instability of the Fermi surface. A magnetic field higher than the metamagnetic critical field suppresses these features and induces strong paramagnon scattering, proving the existence of strong ferromagnetic correlations.

TT 14.15 Tue 18:15 H19

Investigation of Magnetic and Orbital Order in $Ca_3Ru_2O_7$ using Resonant X-ray Diffraction — •Britta Bohnenbuck[1], Jörg Strempfer[2], Ioannis Zegkinoglou[1], Christie Nelson[3], and Bernhard Keimer[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]HASYLAB at DESY, Notkestrasse 85, 22605 Hamburg, Germany — [3]National Synchrotron Light Source, Brookhaven National Laboratory, Upton, New York 11973-5000, USA

We used resonant x-ray diffraction at the L_{II}- and L_{III}- absorption edges of Ru to investigate the bilayered transition metal oxide $Ca_3Ru_2O_7$. This system shows metallic antiferromagnetism between the metal to insulator transition T_{MI}=48K and the antiferromagnetic ordering temperature T_N=56K. In order to learn more about the magnetic and orbital degrees of freedom we performed azimuthal and polarization studies on high quality single crystals both below and above T_{MI} at various reciprocal space positions. Our results are consistent with the magnetic structure proposed by neutron experiments. The magnetic moments are coupled ferromagnetically within the ab-planes but antiferromagnetically between adjacent planes. We also observe a reorientation of the magnetic moment in the ab-plane at T_{MI}. This coincides with a drastic intensity decrease of the magnetic reflection, which vanishes completely at T_N. Our diffraction studies do not give any indication for antiferroorbital order in $Ca_3Ru_2O_7$. However, there might be ferroorbital order as proposed recently by Raman spectroscopy.

TT 14.16 Tue 18:30 H19

Characterization and electronic structure calculations of the antiferromagnetic insulator Ca_3FeRhO_6 — •Volker Eyert[1], Udo Schwingenschlögl[1], Raymond Fresard[2], Antoine Maignan[2], Christine Martin[2], Ninh Nguyen[2], Christian Hackenberger[3], and Thilo Kopp[3] — [1]Institut für Physik, Universität Augsburg, 86135 Augsburg — [2]Laboratoire CRISMAT, UMR CNRS-ENSICAEN(ISMRA) 6508, 14050 Caen Cedex, France — [3]Zentrum für Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, 86135 Augsburg

We investigate the antiferromagnetic insulating nature of Ca_3FeRhO_6 both experimentally and theoretically. Susceptibility measurements reveal a Néel temperature of $T_N \simeq 20\,\mathrm{K}$, and an effective magnetic moment of $5.3\mu_B$ per formula unit. Mössbauer spectroscopy strongly suggests that the Fe ions, located at trigonal prismatic sites, are in a 3+ high spin state. Transport measurements display a simple Arrhenius law, with an activation energy of $\sim 0.2\,\mathrm{eV}$. The experimental results are interpreted with LSDA band structure calculations, which confirm the Fe^{3+} state, the high-spin/low-spin scenario, the antiferromagnetic ordering, and the value for the activation energy.

TT 14.17 Tue 18:45 H19

Electronic structure of the spin chains in $(Ca,Sr)_{14}Cu_{24}O_{41}$ — •Cosima Schuster and Udo Schwingenschlögl — Institu für Physik, Universität Augsburg, 86135 Augsburg

The incommensurate composite systems $(Ca,Sr)_{14}Cu_{24}O_{41}$ are based on three largely independent subsystems, Cu_2O_3 ladders, CuO_2 chains, and electron donor ions. We focus on the electronic properities of the chain subsystem. The crystal structure of the Ca and Sr-rich compound differ in a symmetric or asymmetric alignment of the CuO_2 chains. Substitution of Sr by Ca leads to a transfer of holes from the chains to the ladders. The spin order on the chains likewise depends strongly on the doping and ranges from dimers to antiferromagnetic order. To clarify the electronic structure, we perform calculations based on density functional theory. We present systematic investigations of the local density of states at the chain copper sites and the band structure. The hybridization between the chains, ladders and electron donor ions is found to be negligible. The band structure of coupled corner-shared CuO chains resembles the band structure of the composite system. The chains are well described in terms of two characteristic electronic bands at the Fermi energy.

TT 14.18 Tue 19:00 H19

Interplay of structure and electronic properties in metalorganic spin chain and spin crossover compounds — •Harald O. Jeschke[1], Martin U. Schmidt[2], Tanusri Saha-Dasgupta[3], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Universität Frankfurt, Germany — [2]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, Germany — [3]S.N.Bose National Centre for Basic Sciences, Kolkata, India

We employ a combination of first principles methods to study the electronic and magnetic properties of metalorganic coordination complexes. By combining force field methods and *ab initio* molecular dynamics we construct model structures which are suitable for analysis with precise density functional theory methods. We employ NMTO downfolding to study the relative importance of the interaction paths between the metal centers. In a Cu^{2+} complex that forms a Heisenberg spin 1/2 chain we investigate the possibility of tuning the band width and dimensionality by simple substitutions. In a model Fe^{2+} triazole polymer we investigate the mechanism for the high spin-low spin transition.