TT 49: CE: Spin Systems and Itinerant Magnets 2

Time: Thursday 14:00–18:45 Location: HSZ 03

TT 49.1 Thu 14:00 HSZ 03

Theory of disordered stripes in hole-doped $La_{2-x}Sr_xCoO_4$ — •Matthias Vojta — Technische Universität Dresden, Germany

The compounds $La_{2-x}Sr_xCoO_4$ are isostructural to the 214 family of cuprate superconductors, but remain insulating over a wide doping range. Recently, the x=1/3 compound was found to display a peculiar type of magnetism, with short-ranged static antiferromagnetic order and an hour-glass-like excitation spectrum, not unlike some cuprates. We argue that a scenario of disordered charge stripes, formed by Co^{2+} and Co^{3+} ions, is consistent with the experimental data. In particular, we calculate the magnetic excitation spectrum in the disordered charge background and discuss possible origins of the stripe disorder.

TT 49.2 Thu 14:15 HSZ 03

Vacancies in non-collinear antiferromagnets — •Alexander Wollny[1], Lars Fritz[1], and Matthias Vojta[2] — [1]Institut für theoretische Physik, Universität zu Köln, 50937 Köln — [2]Institut für theoretische Physik, Technische Universität Dresden, 01062 Dresden

We study a single vacancy in the 2D quantum Heisenberg antiferromagnet on the triangular lattice.

We observe that the classical 120 degree ordered state is distorted in the vicinity of the vacancy. We determine that the deviation from the bulk ordered state decays as $1/r^3$ also upon inclusion of quantum corrections controlled in 1/S. The distortion and the $1/r^3$-decay can be understood as the response to a local transversal field generated by the vacancy.

We use both spin wave and Monte Carlo methods to determine the impurity contribution to the uniform susceptibility at zero and finite temperatures respectively.

TT 49.3 Thu 14:30 HSZ 03

Spin dephasing through a nuclear spin bath — •Jasmin V. Jäger, Fabian Güttge, and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

In semiconducting quantum dots the electron spin coherence time is limited due to interactions of the confined electron with its environment. The most relevant decoherence mechanism in such devices is the interaction between the nuclear spins and the central electronic spin. We focus on the time-evolution of a single electron spin interacting with a bath of nuclear spins via the hyperfine interaction. Initially, the nuclear spins are unpolarized and couple to the central spin with a random distribution of hyperfine coupling constants. This central spin model has been solved exactly for a few bath spins by using the exact diagonalization method. By solving equations of motion numerically, we compute the time evolution of the electron spin interacting with a bath of nuclear spins. Because of many-particle correlations the exact equations have to be replaced by approximated equations using a cluster expansion method. In this work, we investigate the quality of the approximation by comparing the results of both methods.

TT 49.4 Thu 14:45 HSZ 03

Valence Bond Crystal on the Hyperkagome Antiferromagnet — •Emil Bergholtz, Andreas Läuchli, and Roderich Moessner — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

We describe our recent work that indicates that the ground state of the antiferromagnetic spin-1/2 Heisenberg model on the highly frustrated, three-dimensional, hyperkagome lattice is a valence bond crystal (VBC) [1]. Performing a series expansion around an arbitrary dimer covering on the hyperkagome we find that a ground state with a huge (72 site) unit cell is selected by the quantum fluctuations. The regularity and favorable energetics of our series expansion establishes the VBC as a serious contender to the earlier spin liquid proposals. We find that the ground state supports many, very low lying, excitations in the singlet sector and that the low energy spinful excitations (spinons and triplons) are effectively confined to various emergent lower-dimensional structures. If applicable to the recently studied sodium iridate compound, $Na_4Ir_3O_8$, this scenario has interesting observable implications, such as spatially anisotropic neutron scattering spectra and possibly multiple finite temperature signatures in the magnetic specific heat due to a multi-step breaking of discrete symmetries. Most saliently, here—as for several proposed states for analogous kagome and pyrochlore magnets—one might expect a clearly resolved Ising transition at relatively high temperature.

[1] E.J. Bergholtz, A.M. Läuchli and R. Moessner, Phys. Rev. Lett., in press (2010) [arXiv:1010.1345]

TT 49.5 Thu 15:00 HSZ 03

Numerical studies of the metallic and insulating phases of a spinless fermion model on a kagome lattice — Aroon O'Brien[1], Frank Pollmann[1], •Satoshi Nishimoto[2], Masaaki Nakamura[3], and Peter Fulde[1,4] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Strasse 38, 01187 Dresden, Germany — [2]IFW Dresden, Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [3]Department of Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan — [4]Asia Pacific Center for Theoretical Physics, Pohang, Korea

Geometrically frustrated models exhibit many fascinating physical properties such as highly degenerate ground states and even the possible existence of fractionally charged excitations. Both phenomena are consequences of the frustrated electronic interactions.

We present a model of spinless fermions on the 2D kagome lattice. In this model a metal-insulator transition occurs as nearest-neighbour interactions are tuned into the strongly correlated regime. We consider the nature of the transition for positive and negative hopping matrix elements; differences between the two cases are attributable to the form of the band structure.

In the insulating phase fractionally charged excitations occur at certain filling factors. An investigation of the dynamical properties of the fractional charges is discussed. Particular focus is given to signatures of the confined collective excitations as observed in numerically calculated spectral densities.

TT 49.6 Thu 15:15 HSZ 03

Thermodynamics of quantum magnets at large S — •Andreas Honecker[1], Mike Zhitomirsky[2], Johannes Richter[3], and Moritz Härtel[3] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Commissariat à l'Energie Atomique, DSM/INAC/SPSMS, Grenoble, France — [3]Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Germany

Experiments demand efficient methods to compute thermodynamic properties of quantum magnets in arbitrary dimensions and with arbitrary interaction geometries as well as spin quantum numbers S at moderate to high temperatures. Using the example of the square lattice, we start by generating reference data for $S \leq 5/2$ by Quantum Monte Carlo simulations and for $S = \infty$ by classical Monte Carlo simulations. Next, we perform a phenomenological scaling analysis with spin quantum number S. We then explore other, mainly semiclassical methods, which avoid expensive numerical simulations. The methods investigated include linearized spin-wave theory, equations of motion for the Green functions, and a Monte-Carlo evaluation of a cumulant expansion in a spin-coherent-states representation. We compare advantages and shortcomings of the different methods.

15 min. break

TT 49.7 Thu 15:45 HSZ 03

Series Expansion Analysis of a Four-Spin Tube — Marcelo Arlego[1] and •Wolfram Brenig[2] — [1]Departamento de Física, Universidad Nacional de La Plata, 1900 La Plata, Argentina — [2]Institute for Theoretical Physics, Technische Universität Braunschweig, 38106 Braunschweig, Germany

We analyze a four-legged anisotropic triangular spin ladder with transverse periodic boundary conditions leading to a frustrated four-spin tube. In the limit of strong rung coupling, and starting from decoupled four-spin plaquettes, we study the zero temperature properties of this quantum spin model, using a series expansion based on the flow equation method. Results will be reported for the ground state energy, as well as for the dispersion of the one- and the two-particle excitations. The effective two-particle interactions will be analyzed and are shown to induce several types of (anti)bound states. In sharp contrast to conventional spin ladders, the renormalized plaquette regime of the four-spin tube is unstable to quantum-phase transitions at finite

leg couplings. These are reported to be of first order and their critical lines will be determined using the density-matrix renormalization group.

TT 49.8 Thu 16:00 HSZ 03

Coherent spin-current oscillations in transverse magnetic fields — •Robin Steinigeweg[1], Stephan Langer[2], Fabian Heidrich-Meisner[2], Ian P. McCulloch[3], and Wolfram Brenig[1] — [1]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany — [2]Department of Physics, Ludwig-Maximilians-Universitaet Muenchen, D-80333 Muenchen, Germany — [3]School of Physical Sciences, The University of Queensland, Brisbane, QLD 4072, Australia

This work addresses coherence properties in the dynamics of spin-currents with components transverse to an externally applied magnetic field for the spin-1/2 Heisenberg chain. We study two cases, first, the linear-response regime at finite temperatures, and second, the real-time dynamics of spin currents during the evolution from initial states with an inhomogeneous transverse magnetization. Apart from a coherent oscillation at the Larmor frequency linked to the integrability of the model we find a second nontrivial collective oscillation at higher frequencies, emerging at low temperatures. We clarify that this oscillation is a many-magnon effect and also becomes coherent at lower temperatures. The collective oscillation frequency and life-time is investigated as a function of temperature and magnetic field, with a satisfying agreement between the two approaches employed.

TT 49.9 Thu 16:15 HSZ 03

Entanglement Spectra and Entanglement Hamiltonians for quantum spin chains — •Ronny Thomale[1], Stephan Rachel[2], Daniel P. Arovas[3], and B. Andrei Bernevig[1] — [1]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA — [2]Department of Physics, Yale University, New Haven, Connecticut 06520, USA — [3]Department of Physics, University of California at San Diego, La Jolla, California 92093, USA

We give a complete definition of the entanglement gap separating low-energy, CFT levels, from high-energy, generic ones, in the "entanglement spectrum" in the momentum cut of gapless quantum spin chains. The approach allows to study the dimerization transition, bulk excitation state counting, and the manifestation of logarithmic CFT corrections purely from the ground state wave function. It provides a new formulation of non-local order in quantum spin chains.

From a different angle, we address the question of how to define Hermitian operators which would serve as entanglement Hamiltonians for spin chains and discuss correspondences and differences between energy and entanglement spectra.

TT 49.10 Thu 16:30 HSZ 03

Derivation of effective microscopic models for the frustrated antiferromagnets Cs_2CuCl_4 and Cs_2CuBr_4 from first principles — •Kateryna Foyevtsova, Ingo Opahle, Yu-Zhong Zhang, Harald O. Jeschke, and Roser Valentì — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

We report on the density functional theory (DFT) investigations of the frustrated triangular-lattice antiferromagnets Cs_2CuCl_4 and Cs_2CuBr_4, which in particular focus on derivation of effective models for the two compounds. The drastic disagreement between the Heisenberg model that we derived for Cs_2CuCl_4 using its X-ray structural data and the experimentally established model motivated us to perform a detailed study of the crystal structure optimization effects on the exchange couplings with a number of exchange-correlation functionals for Cs_2CuCl_4 as well as for Cs_2CuBr_4. We find that, in order to obtain results that are consistent with experiment, one has to consider during the optimization an insulating state, appearing only with a spin-polarized exchange-correlation functional, and electronic correlations (within the LDA+U approach). We will in addition discuss the effect of interlayer couplings as well as longer-ranged couplings in both systems.

As the mixed $Cs_2CuCl_{4-x}Br_x$ ($0 < x < 4$) systems have been gaining a lot of attention recently, we also present some DFT insights on the distribution of either of the halide atoms at various mixing factors.

TT 49.11 Thu 16:45 HSZ 03

Magnetic and structural properties of AFe_4X_2 (A = Y, Sc, Lu, and Zr; X = Ge and Si) — •Nandang Mufti[1], Til Dellmann[2], Philipp Materne[2], Hans H. Klauss[2], Graeme Blake[3], Thomas T. M. Palstra[3], and Christoph Geibel[1] — [1]MPI für Chemische Physik fester Stoffe, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [3]Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands

The compound RFe_4Ge_2 (R = Dy, Ho, Er, Y) have been reported to crystallize with the tetragonal $ZrFe_4Si_2$ structure type and to show interesting magnetic properties. In YFe_4Ge_2, antiferromagnetic ordering with small ordered moment $\sim 0.63\ \mu_B$ occurs simultaneously with a large (2.5 %) first order structural distortion from tetragonal to orthorhombic at 43.5 K. The presence of a large structural distortion despite a weak antiferromagnetic ordering with low T_N and small moments is reminiscent of observations in Fe-arsenides. Here, we will present magnetic and structural properties of AFe_4X_2 (A = Y, Sc, Lu and Zr; X = Ge and Si) based on magnetic susceptibility, specific heat, resistivity and low temperature X-ray diffractometer measurements. Our results indicate the occurrence of a transition in all compounds at critical temperatures between 30 K and 75 K depending on the compounds. There is no systematic relationship between T_N and and the lattice parameters of AFe_4X_2. However, magnetic order and structural distortion seems generally to be connected. The relation between structural, electronic, and magnetic properties will be discussed.

TT 49.12 Thu 17:00 HSZ 03

Mössbauer Spectroscopic Study of Spin and Orbital Order in $FeCr_2S_4$ — •Josefin Engelke[1], Jochen Litterst[1], Alexander Krimmel[2], Alois Loidl[2], Friedrich Wagner[3], Michael Kalvius[3], and Vladimir Tsurkan[2,4] — [1]IPKM TU Braunschweig, Germany, e-mail: j.engelke@tu-bs.de — [2]Experimentalphysik V, Universität Augsburg, Germany, e-mail: alois.loidl@physik.uni-augsburg.de — [3]Physics-Department TU München, Germany, e-mail:kalvius@ph.tum.de — [4]Inst. Applied Physics, Acad. Sciences Moldava, Republic of Moldava

The spinel $FeCr_2S_4$ has been studied intensely in the past for its peculiar magnetic and local structural changes, which are sensitively influenced by the Jahn- Teller properties of Fe^{2+} in tetrahedral sulphur coordination. Recent muon spin rotation data [1] give strong evidence that the collinear ferrimagnetism found below $T_C = 165\ K$ changes to an incommensurate structure below 50 K. Recent high resolution X-ray studies reveal a broadening of Bragg peaks below 50 K and a maximum of mean square displacement around 15 K [2]. Below 10 K orbital order is concluded from specific heat data [2].

We present Mössbauer spectroscopic data taken on the same samples as used in [1, 2]. The influence on spectral shape by changing Jahn-Teller dynamics will be discussed. Special emphasis is placed on the interpretation of the spectra close to the magnetic and orbital transitions.

[1] G. M. Kalvius et al., J. Phys.: Condens. Matter 22, 052205 (2010)
[2] V. Tsurkan et al., Phys. Rev. B81, 184486 (2010)

15 min. break

TT 49.13 Thu 17:30 HSZ 03

Exchange driven phonon splitting in transition-metal monoxides — •Christian Kant[1], Franz Mayr[2], Joachim Deisenhofer[2], and Alois Loidl[2] — [1]TU Wien, Wien, Österreich — [2]Center for Electronic Correlations, Universität Augsburg, Augsburg, Deutschland

The interplay of magnetism and the underlying crystal lattice is a topical issue of condensed-matter physics. It can relieve frustration in the magnetic sector via a spin-driven Jahn-Teller effect in frustrated lattices, leads to novel excitations such as electromagnons in multiferroics, and bears the potential for future applications via magnetodielectric effects. A conceptual understanding of the coupling of spins and phonons is, however, often hampered by the complexity of the interactions. For transition-metal monoxides, which are model systems to study the effects of electronic correlations, a magnetism-induced anisotropy in the lattice response was predicted theoretically. We report optical evidence for a linear dependence of the phonon splitting on the nearest-neighbour exchange coupling in the monoxides MnO, $Fe_{0.92}O$, CoO and NiO. Our results directly confirm the seminal theoretical prediction of a purely exchange induced splitting of the zone-centre optical phonon and pave a new path for the understanding of spin-phonon coupling effects.

TT 49.14 Thu 17:45 HSZ 03

Bose-Einstein Condensation in the Han purple compound:

a high field NMR study — •Steffen Krämer[1], Mladen Horvatic[1], Claude Berthier[1], Raivo Stern[2], and Tsuyoshi Kimura[3] — [1]Laboratoire National des Champs Magnétiques Intenses, CNRS, Grenoble, France. — [2]NICPB, Tallinn, Estonia. — [3]Osaka University, Osaka, Japan.

The quasi-2D, antiferromagnetic exchange coupled spin-1/2 dimer compound $BaCuSi_2O_6$ (Han purple) is considered as a prototype of the magnetic field induced Bose-Einstein Condensation (BEC) of triplet excitations on a lattice. Recently, $BaCuSi_2O_6$ has been claimed to exhibit an unusual reduction of dimensionality of the BEC from 3D to 2D when lowering the temperature, induced by frustration between adjacent planes. However, due to a structural transformation at 90 K, different intradimer exchange couplings and different gaps ($\Delta_B/\Delta_A = 1.16$) exist in every second plane along the c axis. First Nuclear Magnetic Resonance (NMR) experiments have shown that this leads to a population of bosons in the B planes, n_B, much smaller than in A planes in the field range $\Delta_A/g\mu_B < H < \Delta_B/g\mu_B$ where $n_B = 0$ is expected in a model of uncoupled planes. More recently, a better model has been presented, which takes into account both frustration and quantum fluctuations. This leads to a non-zero population n_B of uncondensed bosons in the B plane, increasing quadratically with $(H - H_{c1})$, as compared to the linear dependence of n_A. In our contribution we compare our new NMR results, obtained at high magnetic fields (23-27 T) and low temperatures (50 mK), to these models.

TT 49.15 Thu 18:00 HSZ 03

Vibrating coil magnetometry of the spin ice state in $Ho_2Ti_2O_7$ — •C. Krey[1], S. Legl[1], S. R. Dunsiger[1], C. Pfleiderer[1], J. S. Gardner[2], and J. Roper[3] — [1]Physik Department E21, Technische Universität München, Germany — [2]NIST, Center for Neutron Research, Gaithersburg, Maryland, USA — [3]Los Alamos National Laboratory, Los Alamos, USA

The 'spin ice' model highlights the strong analogy between spin ordering in Ising magnets and proton ordering in ice. Recently, it has been proposed that the excitations may be described in terms of magnetic point defects or emergent magnetic monopoles [1]. The cubic pyrochlore systems $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ are excellent experimental realizations of spin ice, where the local $\langle 111 \rangle$ Ising anisotropy of the rare earth sites in combination with net ferromagnetic interactions give rise to a highly degenerate ground state. The similarities with water ice are the observation of a first order transition terminating in a critical point in the magnetization of $Dy_2Ti_2O_7$ for applied magnetic fields along the global $\langle 111 \rangle$ direction. We report a comprehensive study of the magnetization at mK temperatures of $Ho_2Ti_2O_7$ by means of a vibrating coil magnetometer [2]. We observe considerable qualitative similarities with $Dy_2Ti_2O_7$ but also distinct differences. We consider the role of strong hyperfine interactions associated with Ho compounds.

[1] Ryzhkin, J Exp and Theor Physics 101, 481 (2005), Castelnovo et al., Nature 451, 42 (2008)
[2] Legl et al., Rev. Sci. Instrum. 81, 043911 (2010)

TT 49.16 Thu 18:15 HSZ 03

Probing the local magnetic structure of a quasi-1D cuprate with Resonant Inelastic X-Ray Scattering — Claude Monney[1], Valentina Bisogni[2], Kejin Zhou[1], Roberto Kraus[2], Vladimir Strocov[1], Jochen Geck[2], and •Thorsten Schmitt[1] — [1]Paul Scherrer Institut, Villigen PSI, Switzerland — [2]IFW, Dresden, Germany

The quasi-one-dimensional cuprate Li_2CuO_2 is a prototype edge-sharing chain compound. The Cu^{2+} ions in this strongly correlated material give rise to one spin 1/2 per CuO_4 plaquette with a nearest neighbor Cu-O-Cu bond angle close to 90° implying weak superexchange between Cu spins. As a result, spins order antiferromagnetically between the chains below $T_N \sim 9$K, but ferromagnetically in the chains. We have performed Resonant Inelastic X-ray Scattering (RIXS) at Cu L_3 and O K-resonances at the ADRESS beamline of the Swiss Light Source on this compound. Our momentum resolved RIXS measurements at the Cu L_3-edge allow analyzing orbital excitations with high sensitivity. At the O K-edge, the RIXS spectra display a complicated interplay of low-energy excitations from charge, orbital and lattice degrees of freedom. In particular, we discuss charge transfer related spectral components in the scenario of exotic Zhang-Rice (ZR) singlet and triplet excitations which can be reached in the final state with O K-edge RIXS. The intensity of the ZR features can be related to the thermodynamics of domain walls in one dimension. This establishes RIXS as an excellent probe for investigating local magnetic order.

TT 49.17 Thu 18:30 HSZ 03

The effect of interchain coupling on multipolar phases in quasi-1d quantum helimagnets — •S. Nishimoto[1], S.-L Drechsler[1], R.O. Kuzian[1], J. Richter[2], and J. van den Brink[1] — [1]IFW Dresden, Germany — [2]Universität Magdeburg, Germany

Coupled frustrated spin-1/2 chains in high magnetic fields described within the ferro- antiferromagnetic J_1-J_2 Heisenberg model are studied by DMRG, hard core boson, and spin wave theory approaches. Multipolar phases related to magnon bound states are destroyed (supported) by weak antiferromagnetic (ferromagnetic) interchain couplings J_{ic}. We show that quantum spin nematics might be found for $LiVCuO_4$ whereas for $Li(Na)Cu_2O_2$ it is prevented by a sizeable antiferromagnetic J_{ic}. Also for Li_2ZrCuO_4 with a small antiferromagnetic J_{ic} expected triatic or quartic phases are unlikely, too. The saturation field is found to be strongly affected even by a relatively small J_{ic}.

[1] S. Nishimoto, S.-L. Drechsler, R.O. Kuzian, J. Richter, and J. van den Brink, arXiv:1005.5500v2.
[2] S. Nishimoto, S.-L. Drechsler, R.O. Kuzian, J. van den Brink, J. Richter, W.E.A. Lorenz, Y. Skourski, R. Klingeler, B. Büchner, arXiv:1004.3300v2.
[3] S.-L. Drechsler, S. Nishimoto, R.O. Kuzian, J. Malek, W.E.A. Lorenz, J. Richter, J. van den Brink, M. Schmitt, H. Rosner, arXiv:1006.5070v2.