TT 50: Correlated Electrons: Frustrated Magnets - Low-Dimensional Systems

Time: Wednesday 15:00–18:00 Location: HSZ 304

TT 50.1 Wed 15:00 HSZ 304

Quantum Monte Carlo simulations of a frustrated ladder in the dimer basis — •Andreas Honecker[1] and Stefan Wessel[2] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, Université de Cergy-Pontoise, France — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen University, Germany

Frustrated quantum spin systems are notorious for the infamous "sign problem" that prohibits efficient Quantum Monte Carlo simulations in relevant temperature regions. However, the sign problem is basis dependent. Indeed, recent works [1,2] have shown that passing to a rung-dimer basis eliminates the sign problem for the case of a highly frustrated two-leg spin-1/2 ladder where diagonal couplings are equal to the leg couplings. Here we generalise this result to the case where the two couplings along the legs remain antiferromagnetic but are in general different. We find that although the sign problem re-appears in general, it remains sufficiently mild throughout the phase diagram of the frustrated ladder such that efficient Quantum Monte Carlo simulations can be performed, yielding accurate results for thermodynamic quantities such as magnetic susceptibility and specific heat.

[1] A. Honecker, S. Wessel, R. Kerkdyk, T. Pruschke, F. Mila, B. Normand, Phys. Rev. B **93** (2016) 054408

[2] F. Alet, K. Damle, S. Pujari, Phys. Rev. Lett. **117** (2016) 197203

TT 50.2 Wed 15:15 HSZ 304

Effective spin-Hamiltonian for the 1D Hubbard model at arbitrary coupling strength — Rolf Schumann[1] and •Stefan-Ludwig Drechsler[2] — [1]Institut für Theoretische Physik, TU Dresden, D-01062,Germany — [2]Institute for Solid State Theory, Leibniz-Instiitute IFW-Dresden, D-01171 Dresden. Germany

Using exact diagonalization analytical results for small clusters (dimers, trimers and tetramers) we derive an approximate *effective* spin-Hamiltonian valid for any ratio $u = U/t$, where U denotes the on-site Coulomb repulsion and t is the nearest neighbor (NN)-transfer integral. Thereby we present analytical results for the first, second (NNN), third neighbor exchange integrals $J_1 \gg J_2 \gg J_3$, respectively, and also for the leading cyclic quartic (four spin) exchange term. All interaction parameters are smooth monotonous functions of u without any artificial divergency at $u = 4$ or even $u = 0$ as in other methods based on perturbational theory. Our results compare well with those for the NN (analytical expression) and the NNN (numerical data are available in the limit $u \geq 4$, only) exchange integrals J_1 and J_2, respectively, obtained within the flow-equation technique [1,2]. Possible applications for "conducting" polymers and spin-Peierls systems being in the intermediate coupling regime are briefly disussed.

[1] S.A. Hamerla *et al.*, Phys. Rev. B **82**, 235117 (2010)

[2] S.A. Hamerla and G. Uhrig, unpublished.

TT 50.3 Wed 15:30 HSZ 304

Ground-state phase diagram of the $J_1 - J_1' - J_2$ chain — •Cliò Efthimia Agrapidis[1,2], Stefan-Ludwig Drechsler[1], Jeroen van den Brink[1,2], and Satoshi Nishimoto[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — [2]Department of Physics, Technical University, Dresden, 01069 Dresden, Germany

Quasi one-dimensional (1D) frustrated systems, despite their simple structure, are at the center of attention as a playground for novel ground states that can emerge from frustration and strong quantum fluctuations due to low dimensionality. Motivated by the extensive interest in this field and by recent experimental results, we study the one-dimensional Heisenberg model with dimerized nearest-neighbor ferromagnetic ($J_1, J_1' < 0$) and next-nearest-neighbor antiferromagnetic ($J_2 > 0$) couplings using the spin-wave theory and the density-matrix renormalization group technique. Based on the numerical calculations of total spin, spin gap, equal-time spin-spin correlation functions, and Tomonaga-Luttinger spin exponent, we present the ground-state phase diagram in the space of frustration ratio ($\alpha = J_2/|J_1|$) and dimerization degree ($\beta = J_1'/J_1$). We find a first-order transition between fully-polarized FM and incommensurate singlet state at $\alpha_c = (\beta/2)/(1+\beta)$ and we suggest the existence of a crossover between an AKLT-type valence bond solid state and a frustration-induced dimerized state in the gapped phase. In the absence of dimerization ($\beta = 1$), the spin gap opens at $1/4 < \alpha \lesssim 1.52$. Relevance to the quasi-one-dimensional frustrated compounds $LiCuSbO_4$ and $Rb_2Cu_2Mo_3O_{12}$ is also discussed.

TT 50.4 Wed 15:45 HSZ 304

Dynamic structure factor of disordered quantum spin ladders — •Max Hörmann and Kai Phillip Schmidt — Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

We investigate the zero-temperature dynamic structure factor of a two-leg spin-1/2 Heisenberg ladder with quenched disorder relevant for inelastic neutron scattering. To this end we apply perturbative continuous unitary transformations about the limit of isolated rungs using a white-graph expansion [1] to derive the physical properties of the elementary triplon excitations of the disordered spin ladder in the thermodynamic limit. Here we study bimodal disorder on rungs and legs realizable in experiments by intential doping of existing spin-ladder compounds. We focus on the one-triplon properties which we calculate with high precision in the weakly-coupled rung regime. We observe that the dynamic structure factor displays characteristic differences in rung and leg disorder.

[1] K. Coester and K.P. Schmidt, Phys. Rev. E 92, 022118 (2015).

TT 50.5 Wed 16:00 HSZ 304

Critical behavior of quantum magnets with long-range interactions in the thermodynamic limit — •Sebastian Fey — Lehrstuhl für Theoretische Physik I, Staudtstraße 7, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Quasi-particle properties of quantum magnets with long-range interactions are investigated by high-order linked-cluster expansions in the thermodynamic limit. It is established that perturbative continuous unitary transformations on white graphs are a promising and flexible approach to treat long-range interactions in quantum many-body systems. We exemplify this scheme for the one-dimensional transverse-field Ising chain with long-range interactions. For this model the elementary quasi-particle gap is determined allowing to access the quantum-critical regime including critical exponents and multiplicative logarithmic corrections for the ferro- and antiferromagnetic case.

TT 50.6 Wed 16:15 HSZ 304

The dynamics of linarite: Observations of magnetic excitations — Kirrily C. Rule[1], Britta Willenberg[2,3], Markus Schäpers[4], Anja U.B. Wolter[4], Stefan L. Drechsler[4], Georg Ehlers[5], Alan Tennant[5], Richard Mole[1], Jason Gardner[6,7], •Stefan Süllow[2], and Satoshi Nishimoto[4,8] — [1]ANSTO, Kirrawee, Australia — [2]IPKM, TU Braunschweig, Braunschweig, Germany — [3]HZB für Materialien und Energie, Berlin, Germany — [4]IFW Dresden, Dresden, Germany — [5]ORNL, Oak Ridge, USA — [6]NSRRC, Hsinchu, Taiwan — [7]CCMS, National Taiwan University, Taipei, Taiwan — [8]Dept. Physics, TU Dresden, Dresden, Germany

Here we present inelastic neutron scattering measurements from the frustrated, quantum spin-1/2 chain material linarite, $PbCuSO_4(OH)_2$. Time of flight data, taken at 0.5 K and zero applied magnetic field reveals low-energy dispersive spin wave excitations below 1.5 meV both parallel and perpendicular to the Cu-chain direction. From this we confirm that the interchain couplings within linarite are around 10 % of the nearest neighbour intrachain interactions. We analyse the data within both linear spin-wave theory and density matrix renormalisation group theories and establish the main magnetic exchange interactions and the simplest realistic Hamiltonian for this material.

15 min. break.

TT 50.7 Wed 16:45 HSZ 304

DMRG simulations of SU(N) Heisenberg models using a million of states — •Andreas Weichselbaum[1], Sylvain Capponi[2], Andreas Läuchli[3], Alexei Tsvelik[4], and Philippe Lecheminant[5] — [1]Ludwig Maximilians University, Munich, Germany — [2]CNRS Toulouse, Université Paul Sabatier, France — [3]University of Innsbruck, Austria — [4]Brookhaven National Laboratory, Upton, NY, USA — [5]Université de Cergy Pontoise, France

The density matrix renormalization group (DMRG) is applied to SU(N) symmetric Heisenberg chains and ladders while fully exploiting the underlying SU(N) symmetry. Since these models can be motivated from symmetric N-band fermionic models, it is immediately

clear that the numerical complexity of simulating SU(N) symmetric models grows exponentially in N. Nevertheless in the presence of symmetry this exponential growth is largely transferred to the symmetry multiplets in that the largest multiplets that appear in a typical simulation grow exponentially in size like 10^{N-1}. Therefore while keeping a moderate number of multiplets, the full state space dimension required for converged results can quickly reach a million of states. Recent results on Heisenberg ladders with $N \leq 5$ and varying rung coupling are discussed and contrasted to existing literature.

TT 50.8 Wed 17:00 HSZ 304

Unconventional nematic state in the frustrated and anisotropic spin-chain cuprate $LiCuSbO_4$ — •Satoshi Nishimoto[1,2], Hans-Joachim Grafe[1], Margarita Iakovleva[1,3], Evgeniia Vavilova[1,3], Alexey Alfonsov[1], Mihai-I. Sturza[1], Helge Rosner[4], Johannes Richter[5], Ulrich Rössler[1], Stefan-Ludwig Drechsler[1], Vladislav Kataev[1], and Bernd Büuchner[1,2] — [1]IFW Dresden, Germany — [2]TU Dresden, Germany — [3]Zavoisky Physical Technical Institute, Kazan, Russia — [4]MPI-cPfS, Dresden, Germany — [5]U. Magdeburg, Germany

Modern theories of quantum magnetism predict exotic multipolar states in frustrated spin-1/2 Heisenberg chains with ferromagnetic nearest-neighbor (NN) inchain exchange in high magnetic fields. Experimentally these states remained elusive so far. Here we report the evidence for a long-sought magnetic field-induced nematic state arising above a field of $\sim 13\,\mathrm{T}$ in the edge-sharing chain cuprate $LiCuSbO_4$. This interpretation is based on the observation of a field induced spin-gap in the measurements of the ^{7}Li NMR spin relaxation rate T_1^{-1} as well as a contrasting field-dependent power-law behavior of T_1^{-1} vs. T and is further supported by static magnetization and ESR data. An underlying theoretical microscopic approach favoring a unconventional nematic scenario is based essentially on the NN XYZ exchange anisotropy within a model for frustrated spin-1/2 chains. It is investigated by the DMRG technique. The employed exchange parameters are justified qualitatively by electronic structure calculations for $LiCuSbO_4$.

TT 50.9 Wed 17:15 HSZ 304

Structural and Magnetic Properties of the trirutile-type 1D Heisenberg Antiferromagnet $CuTa_2O_6$ — •Aleksandr Golubev[1], R. E. Dinnebier[1], A. Schulz[1], R. K. Kremer[1], H. Langbein[2], A. Senyshyn[3], J. M. Law[4], Th. Hansen[5], E. E. Gordon[6], and M.-H. Whangbo[6] — [1]MPI for Solid State Research, D-70569 Stuttgart, Germany — [2]Institut für Anorganische Chemie der TUD, D-01062 Dresden, Germany — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), TUM, D-85747 Garching, Germany — [4]Dresden High Magnetic Field Laboratory (HLD), D-01314 Dresden-Rossendorf, Germany — [5]ILL, B.P. 156, 38043 Grenoble, France — [6]Department of Chemistry, NCSU, Raleigh, North Carolina 27695-8204, USA

Polycrystalline samples of $CuTa_2O_6$ prepared by low-temperature decomposition of Cu-Ta-oxalate precursors at room temperature crystallize with a monoclinically distorted trirutile structure type. By detailed high temperature x-ray and neutron powder diffraction studies we detected a structural phase transition to the tetragonal trirutile structure-type at 503(3) K. The structural phase transition was ascertained by Raman scattering. GGA+U DFT calculations of the spin exchange parameters, magnetic susceptibility and isothermal magnetization measurements constitute $CuTa_2O_6$ as new 1D Heisenberg chain with predominant afm nearest neighbor exchange interaction $J_{\mathrm{nn}} \approx 50$ K. Heat capacity and low temperature high intensity neutron powder diffraction studies could not find long range order down to 0.4K.

TT 50.10 Wed 17:30 HSZ 304

Intertwined nematic orders in a frustrated ferromagnet — •Yasir Iqbal[1], Pratyay Ghosh[2], Rajesh Narayanan[3], Brijesh Kumar[2], Johannes Reuther[4,5], and Ronny Thomale[1] — [1]Institute for Theoretical Physics, Universität Würzburg, 97074 Würzburg, Germany — [2]Jawaharlal Nehru University, New Delhi 110067, India — [3]Indian Institute of Technology Madras, Chennai 600036, India — [4]Freie Universität Berlin, 14195 Berlin, Germany — [5]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

We investigate the quantum phases of the frustrated spin-$\frac{1}{2}$ J_1-J_2-J_3 Heisenberg model on the square lattice with ferromagnetic J_1 and antiferromagnetic J_2 and J_3 interactions. Using the pseudo-fermion functional renormalization group technique, we find an intermediate paramagnetic phase located between classically ordered ferromagnetic, stripy antiferromagnetic, and incommensurate spiral phases. We observe that quantum fluctuations lead to significant shifts of the spiral pitch angles compared to the classical limit. By computing the response of the system with respect to various spin rotation and lattice symmetry-breaking perturbations, we identify a complex interplay between different nematic spin states in the paramagnetic phase. While retaining time-reversal invariance, these phases either break spin-rotation symmetry, lattice-rotation symmetry, or a combination of both. We therefore propose the J_1-J_2-J_3 Heisenberg model on the square lattice as a paradigmatic example where different intimately connected types of nematicities emerge in the same model.

TT 50.11 Wed 17:45 HSZ 304

Topological quantum paramagnet in a quantum spin ladder — •Darshan G. Joshi and Andreas P. Schnyder — Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany

Recently, it has been shown that analogs of quantum Hall systems could be realized in quantum magnets. Most of these works have focused on the symmetry broken phases in magnetic systems. In this work, we consider the dimer-quantum-paramagnetic phase of a S=1/2 quantum spin ladder, which does not break any symmetry of the parent Hamiltonian. We show that in the presence of Dzyaloshinskii-Moriya interaction and external magnetic field the paramagnetic phase is actually split into a topologically trivial and a topologically non-trivial phase. We calculate the winding number and the end-states in this topologically non-trivial phase. The topological aspect is a consequence of the reflection symmetries present in the model and other models with similar properties may also realize the same physics.