TT 29: Frustrated Magnets: General

Time: Wednesday 9:30–13:15 Location: HSZ 201

TT 29.1 Wed 9:30 HSZ 201

Possible stress-driven spiral-to-Néel transition in the triangular antiferromagnet $PdCrO_2$ — •Nina Stilkerich[1,2], Seunghyun Khim[2], Andrew Mackenzie[2,3], Jochen Geck[1], and Clifford Hicks[2,4] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [3]Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom — [4]School of Physics and Astronomy, University of Birmingham, Birmingham B15 2TT, United Kingdom

$PdCrO_2$ is a triangular antiferromagnet that undergoes a transition from a double-q to single-q magnetic structure under moderate uniaxial stress [1]. Due to a high sensitivity of the magnetic anisotropy to uniaxial stress, another transition from spiral order to a linear antiferromagnetic structure is predicted for higher stress of about 1 GPa [1]. We performed stress-strain measurements on $PdCrO_2$ and were able to identify the double- to single-q transition as a jump in strain. We report the discovery of an additional transition under higher stress, which might be the spin spiral to Néel transition suggested previously.
[1] D. Sun et al., New J. Phys. 23, 123050 (2021)

TT 29.2 Wed 9:45 HSZ 201

Thermodynamic study of the partially polarized state of the sawtooth chain atacamite, $Cu_2Cl(OH)_3$ — Leonie Heinze[1], Tommy Kotte[2], Albin de Muer[3], Sven Luther[2,4], Andrew Ammerlaan[5], Uli Zeitler[5], Anja U.B. Wolter[6], Bernd Büchner[6], Kirrily C. Rule[7], Hannes Kühne[2], and •Stefan Süllow[1] — [1]TU Braunschweig, Braunschweig, Germany — [2]HLD, HZ Dresden-Rossendorf, Germany — [3]LNCMI, CNRS, Grenoble, France — [4]TU Dresden, Dresden, Germany — [5]HFML, Radboud University, Nijmegen, The Netherlands — [6]ANSTO, Lucas Heights, Australia — [7]IFW Dresden, Dresden, Germany

Recently, the natural mineral atacamite, $Cu_2Cl(OH)_3$, has been established as a unique model compound of the $S = 1/2$ quantum sawtooth chain with a dominant magnetic exchange $J \sim 360\,\mathrm{K}$ along the chain spine and $J' \sim 102\,\mathrm{K}$ within the sawteeth [1]. Residual interchain couplings of a few Kelvin drive atacamite into an antiferromagnetic (AFM) ground state below $T_N = 8.4\,\mathrm{K}$. The AFM phase is suppressed in magnetic fields of $\sim 30\,\mathrm{T}$. Upon suppression of AFM order, the magnetization becomes plateau-like close to $M_{sat}/2$.

By now, we have been able to study the magnetic phase diagram up into the unusual partially polarized state by means of specific heat. Here, we present a corresponding study and present evidence for quantum critical behavior occuring upon suppression of AFM order.
[1] L. Heinze *et al.*, Phys. Rev. Lett. **126**, 207201 (2021).

TT 29.3 Wed 10:00 HSZ 201

Weakly coupled triangles forming a star lattice in an organic-inorganic copper sulfate — •Oleg Janson[1], Ulrich K. Rössler[1], and Hajime Ishikawa[2] — [1]Leibniz IFW Dresden, Germany — [2]ISSP, University of Tokyo, Japan

The recently synthesized organic-inorganic copper sulfate $[(CH_3)_2(NH_2)]_3[Cu_3(OH)(SO_4)_4]\cdot 0.24H_2O$ has been proposed as a material realization of the $S = \frac{1}{2}$ star lattice model [1]. We report high-field magnetization measured on powder samples showing a broad plateau at $\frac{1}{3}$ of the saturation magnetization. Full saturation was reached at about 105 T in a destructive pulsed-field experiment. Low-field and low-temperature measurements on single crystals show no indications of magnetic ordering and reveal a sizable anisotropy of magnetization. Density-functional-theory (DFT) calculations indicate the relevance of two inequivalent exchanges J_T and J_D with $J_\mathrm{T} \gg J_\mathrm{D}$, placing this material in the limit of weakly coupled triangles. Anisotropic components of J_T were estimated by noncollinear DFT+U calculations. We demonstrate that a simple model of isolated triangles accounts for the thermodynamic behavior of this compound.
[1] M. Sorolla *et al.*, J. Am. Chem. Soc. **142**, 5013 (2020)

TT 29.4 Wed 10:15 HSZ 201

Temperature-dependent transitions of the rare-earth delafossite $NaGdS_2$ — •Justus Grumbach[1], Mathias Doerr[1], Ellen Haeussler[2], and Sergey Granovsky[1] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Fakultät für Chemie und Lebensmittelchemie, Technische Universität Dresden, 01062 Dresden, Germany

Rare-earth delafossites are materials containing ideal triangular magnetic planes, which are frustrated. Due to their properties, rare-earth delafossites are promising candidates for a QSL ground state. In recent years this state occured in some S=$\frac{1}{2}$-delafossites with transitions in the mK range.
Now a number of own new measurements were made on $NaGdS_2$ single crystals. This delafossite with magnetic Gd^{3+} ions, which has been extensively investigated for the first time, is of special interest due to the pure spin moment J=S=$\frac{7}{2}$. Measurements of several different thermodynamic and magnetic properties were performed on very small samples (size $\sim \mu$m) down to lowest temperatures (40 mK).
Essential physical data could be extracted, which show correspondingly a AFM-groundstate below ∼250 mK, which is kind of expected. An additionally investigated modification at 60 K, indicating an anisotropy in the system, is still under theoretical debate and will form a main part of the talk.

TT 29.5 Wed 10:30 HSZ 201

Study of $CoNb_2O_6$ magnetic properties from first principles — •Amanda Konieczna[1], Kira Riedl[1], Roser Valenti[1], and Radu Coldea[2] — [1]Goethe-Universität, Frankfurt am Main, Germany — [2]University of Oxford, Oxford, England

The quasi-one-dimensional ferromagnet $CoNb_2O_6$ offers an interesting playground to investigate the interplay of anisotropic magnetic interactions in real materials. A variety of magnetic models was proposed for this material, including longer-range Heisenberg exchange, dominant anisotropic Ising and bond-dependent Kitaev-type magnetic interactions.

In this talk, we discuss our theoretical approach to extract the magnetic exchange in $CoNb_2O_6$. We first obtain material-specific hoppings from ab-initio methods and proceed by moving from a description in terms of the Hubbard model to the Spin Hamiltonian using exact diagonalization and perturbation theory. Finally, we will discuss how our results fit into the picture of available results for this system, both on the theoretical and experimental side.

We gratefully acknowledge funding by the DFG (German Research Foundation): QUAST-FOR5249 - 449872909 (Project TP4).

TT 29.6 Wed 10:45 HSZ 201

Valence bond solid state in explicitly dimerized chain with magnetic frustration — •Jędrzej Wardyn[1], Satoshi Nishimoto[1,2], and Cliò Efthimia Agrapidis[3] — [1]IFW Dresden, 01069 Dresden, Germany — [2]TU Dresden, 01062 Dresden, Germany — [3]Faculty of Physics, University of Warsaw, Pasteura 5, 02093 Warsaw, Poland;

We consider the spin-1/2 dimerized frustrated ferromagnetic (FM) $J_1{-}J_1'{-}J_2$ model, with $J_1, J_1' < 0$ FM first neighbours coupling and $J_2{>}0$ antiferromagnetic second neighbors coupling. This model serves as a minimal model for $LiCuSbO_4$ and $Rb_2Cu_2Mo_3O_{12}$. We introduce the frustration parameter $J_2/|J_1|{=}\alpha$ and the dimerization parameter $J_1'/J_1{=}\beta$. There are two special limits of dimerization: fully dimerized at $\beta{=}0$ and the undimerized $J_1{-}J_2$ model at $\beta{=}1$. Earlier studies have identified phases featured in the special limits as valence bond solid with a finite spin gap for $\beta{=}1$ and a Haldane-like state for $\beta{=}0$. For our model, the spin gap and phase diagram was investigated in a 2017 study by Agrapidis *et al.* [1]. Thanks to new insight, we revisit these results with applying new boundary conditions, which allow us to correctly estimate the spin gap which was previously underestimated. We compute the spin gap, the string order parameter (SOP), and dimer-dimer correlations using the density matrix renormalization group method (DMRG). We prove that the model features a VBS state. Our results allow us to determine this state as $\mathcal{D}_3$-VBS state adiabatically connected to the Haldane-like state in the limit of $\beta{=}0$.
[1] C. E. Agrapidis *et al.*, Phys. Rev. B, 95, 220404 (2017).

TT 29.7 Wed 11:00 HSZ 201

The effect of nonlocal electronic correlations on different lattice geometries - A dynamical vertex approximation study

— •Marvin Leusch[1], Andreas Hausoel[2], Alessandro Toschi[3], Giorgio Sangiovanni[4], and Georg Rohringer[1] — [1]Universität Hamburg, Hamburg, Germany — [2]IFW Dresden, Germany — [3]Julius-Maximilians-Universität Würzburg, Würzburg, Germany — [4]TU Wien, Vienna, Austria

In the last decades, dynamical mean-field theory (DMFT) has become a standard tool for describing strongly correlated electron systems. It captures all purely local correlations effects and, hence, provides exact results in the limit of infinite coordination number and thus spacial dimensions. For finite dimensional systems, it neglects nonlocal correlation effects which are captured by diagrammatic extensions of DMFT such as the dynamical vertex approximation (DΓA). In our work, we analyze the three dimensional Hubbard model on various lattice types to investigate the effect of different coordination numbers on local and nonlocal correlations. In particular, we study the magnetic phase diagram of the Hubbard model on a simple cubic (sc), body-centered cubic (bcc) and face-centered cubic (fcc) lattice within DΓA and compare their transition temperatures to magnetically ordered states to corresponding DMFT results. Our numerical findings demonstrate, that the nonlocal correlations of DΓA generally reduce the size of the ordered region with respect to DMFT while the actual magnitude of this reduction depends on the specific lattice type and, in particular, on the coordination number.

15 min. break

TT 29.8 Wed 11:30 HSZ 201

Systematic analysis of diagonal ordering patterns in bosonic lattice models with algebraically decaying density-density interactions — •Jan Alexander Koziol[1], Antonia Duft[1], Giovanna Morigi[2], and Kai Phillip Schmidt[1] — [1]Department of Physics, Staudtstraße 7, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Theoretical Physics, Saarland University, Campus E2.6, D-66123 Saarbrücken, Germany

We propose a general approach to analyse diagonal ordering patterns in bosonic lattice models with algebraically decaying density-density interactions on arbitrary lattices. The key idea is a systematic search for the energetically best order on all unit cells of the lattice up to a given extent. Using resummed couplings we evaluate the energy of the ordering pattern in the thermodynamic limit using finite unit cells. We apply the proposed approach to the atomic limit of the extended Bose-Hubbard on a triangular lattice at fillings $f = 1/2$ and $f = 1$. We investigate the ground-state properties of the antiferromagnetic long-range Ising model on the triangular lattice and determine a six-fold degenerate plain-stripe phase to be the ground state for finite decay exponents. We also probe the classical limit of the Hamiltonian describing Rydberg atom arrangements on the sites and links of the Kagome lattice.

TT 29.9 Wed 11:45 HSZ 201

Phases of the spin-1/2 Heisenberg antiferromagnet on the diamond-decorated square lattice in a magnetic field — •Nils Caci[1], Katarína Karľová[2], Taras Verkholyak[3], Jozef Strečka[2], Stefan Wessel[1], and Andreas Honecker[4] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]Department of Theoretical Physics and Astrophysics, P.J. Šafárik University, Košice, Slovakia — [3]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, L'viv, Ukraine — [4]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, CY Cergy Paris Université, France

The spin-1/2 Heisenberg antiferromagnet on the highly frustrated diamond-decorated square lattice is a spin system of orthogonal spin dimers that features various ground-state phases, consisting of extended monomer-dimer and dimer-tetramer ground states as well as a ferrimagnetic regime. By using a combination of density matrix renormalization group (DMRG), exact diagonalization, as well as unbiased sign-problem free quantum Monte Carlo (QMC) methods, we investigate this system in the presence of a finite magnetic field. We find at high magnetic fields the emergence of a spin-canted phase, with continuously rising magnetization, as well as the fully polarized paramagnetic phase. At intermediate field strength, we identify the presence of a first-order quantum phase transition line between a ferrimagnetic phase and the monomer-dimer regime, which extends to finite temperatures and terminates in a line of critical points belonging to the Ising universality class.

TT 29.10 Wed 12:00 HSZ 201

Ground-state degeneracy and magneto-thermodynamics of the spin-1/2 Heisenberg antiferromagnet on the diamond-decorated square lattice — •Andreas Honecker[1], Nils Caci[2], Taras Verkholyak[3], Katarína Karľová[4], Stefan Wessel[2], and Jozef Strečka[4] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, CY Cergy Paris Université, France — [2]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [3]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, L'viv, Ukraine — [4]Department of Theoretical Physics and Astrophysics, P.J. Šafárik University, Košice, Slovakia

The spin-1/2 Heisenberg antiferromagnet on the diamond-decorated square lattice exhibits a rich ground-state phase diagram in a magnetic field [1]. We investigate the thermodynamic properties of this model using a combination of analytical and numerical methods, including full diagonalization up to effectively $N = 30$ sites. We focus in particular on the vicinity of a "dimer-tetramer" phase at low magnetic fields that maps to a classical dimer model on the square lattice and retains a macroscopic ground-state ddegeneracy in a magnetic field. We discuss the consequences of this degeneracy for the thermodynamic and magnetocaloric properties of the system.

[1] N. Caci, K. Karlova, T. Verkholyak, J. Strečka, S. Wessel, A. Honecker, preprint arXiv:2210.15330

TT 29.11 Wed 12:15 HSZ 201

Thermodynamics of the frustrated Heisenberg model on the truncated hexagonal lattice — •Adrien Reingruber[1], Nils Caci[2], and Stefan Wessel[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen University, Aachen, Germany

The thermodynamical properties of the spin-1/2 Heisenberg antiferromagnet on the truncated hexagonal lattice are studied using trimer-based cluster quantum Monte Carlo simulations. The system consists of an arrangement of spin-trimers on a honeycomb lattice with dimer couplings interconnecting neighboring trimers. The physics of this frustrated quantum spin system is investigated for different spin-coupling strengths. The severeness of the quantum Monte Carlo sign problem with respect to the single-site, dimer and trimer basis is examined. In the parameter regime of weakly coupled trimers an effective spin-1/2 Hamiltonian can be derived to describe the low-temperature physics. This effective model yields antiferromagnetic effective spin-1/2 trimer-spin interactions with bond-dependent coupling strengths. Unbiased quantum Monte Carlo simulations confirm the validity of the effective model within the low-temperature regime.

TT 29.12 Wed 12:30 HSZ 201

Another exact ground state of a 2D quantum antiferromagnet — Pratyay Ghosh, •Tobias Müller, Jannis Seufert, and Ronny Thomale — Julius-Maximilians-Universität, Würzburg, Germany

We present the exact dimer ground state of a quantum antiferromagnet on the maple-leaf lattice. A coupling anisotropy for one of the three inequivalent nearest-neighbor bonds is sufficient to stabilize the dimer state. Together with the Shastry-Sutherland Hamiltonian, we show that this is the only other model with an exact dimer ground state for all two-dimensional lattices with uniform tilings. We futhermore discuss the stability of this ground state from the perspective of perturbation theory.

TT 29.13 Wed 12:45 HSZ 201

Bound states and plateaus: Magnetization behavior of the maple leaf lattice — •Jannis Seufert, Pratyay Ghosh, Tobias Müller, and Ronny Thomale — Julius-Maximilians-Universität, Würzburg, Germany

Recently, the maple leaf lattice equipped with a Heisenberg-Hamiltonian was shown to exhibit an analytically exact antiferromagnetic dimer ground state analogous to the better known Shastry-Sutherland model. Anticipating that its even stronger frustration will lead to both familiar and exotic magnetic behavior, we present the calculation of magnetization plateaus in the maple leaf model with Ising- and Heisenberg-spins. For the latter, this is achieved within a perturbation theory of magnetic excitations incorporating triplet-triplet interactions and correlated hopping, which promotes the emergence of bound states.

TT 29.14 Wed 13:00 HSZ 201

Exact analytical solutions of a distorted spin-1/2 tetrahedron with ring exchange — Rolf Schumann[1] and •Stefan-Ludwig Drechsler[2] — [1]TU-Dresden, D-1169 Dresden, Germany — [2]IFW-Dresden, D-1169 Dresden, Germany

We present exact analytical solutions for the eigenvalues of a general spin-1/2 Hamiltonian with 6 bilinear (Heisenberg) J_i and 3 ring exchange K_i couplings. Focusing on the experimentally interesting orthorhombically, tetragonally, trigonally and non-distorted ideal tetrahedra (ITH) we consider their thermodynamic properties as the magnetization M, susceptibility, entropy, and specific heat at any temperature T and external magnetic field H and derive from the magnetization steps $M(H)$ at high-fields and low-T the saturation field H_s, the critical ferrimagnetic field H_{c1}, and the width of the corresponding plateau as a function of the cyclicity . As a result we find enhanced H_s and lowered H_{c1} values with increasing ring exchange $K > 0$ due to the reduced frustration. We present exact mapping equations to extract the relevant exchange integrals J_i and K_i from experimentally observed transition energies and provide an analytical mapping of the single-band Hubbard model on the ITH valid at any coupling strength U/t, where U is the onsite Coulomb repulsion and t the NN-hopping integral. The experimental situations with respect to the magnitude and sign of $\kappa = J/K$ for $Cu_2Te_2OBr_2$, Cu_2OSeO_3, and $Cu_4X_6L_4$ with X=Cl,Br and L being various ligands are briefly discussed.