TT 23: Frustrated Magnets - General

Time: Wednesday 15:00–18:30 Location: H22

TT 23.1 Wed 15:00 H22

Numerical linked cluster expansion for magnetostriction of frustrated magnets — •Alexander Schwenke and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany

Thermodynamic and magnetoelastic properties of the frustrated J-K-Γ quantum spin model for proximate Kitaev magnets on the honeycomb lattice in a finite magnetic field $\vec{B}$ are studied using the numerical linked cluster expansion (NLCE) [1]. Calculations are performed on clusters of sizes up to $\sim \mathcal{O}(11)$. First, the specific heat and the magnetization are analyzed for in- as well as for out-of-plane configurations of $\vec{B}$. Second, we present results of the linear magnetostriction coefficient $\lambda(\vec{B}, T)$. This displays strongly anisotropic behavior and a clear indication for a field-induced transition. Third, employing exchange parameters as proposed for the proximate quantum spin-liquid (QSL) candidate α-$RuCl_3$, we show that our results for λ are very similar to recently observed experimental data [2] on this material.

[1] M. Rigol et al., Phys. Rev. Lett. **97**, 187202 (2006)
[2] V. Kocsis et al., Phys. Rev. B **105**, 094410 (2022)

TT 23.2 Wed 15:15 H22

Dynamic structure factor of the antiferromagnetic Kitaev model in large magnetic fields — •Andreas Schellenberger, Max Hörmann, and Kai Phillip Schmidt — FAU Erlangen-Nürnberg, Erlangen, Deutschland

We investigate the dynamic structure factor of the antiferromagnetic Kitaev honeycomb model in a magnetic field by applying perturbative continuous unitary transformations about the high-field limit. One- and two-quasi-particle properties of the dressed elementary spin flip excitations of the high-field polarized phase are calculated which account for most of the spectral weight in the dynamic structure factor. We discuss the evolution of spectral features in these quasi-particle sectors in terms of one-quasi-particle dispersions, two-quasi-particle continua, the formation of anti-bound states, and quasi-particle decay. In particular, a comparably strong spectral feature above the upper edge of the upmost two-quasi-particle continuum represents three anti-bound states which form due to nearest-neighbor density-density interactions.

[1]arXiv:2203.13546 [cond-mat.str-el]

TT 23.3 Wed 15:30 H22

Fractionalized quantum criticality in spin-orbital liquids from field theory beyond the leading order — Shouryya Ray[1], Bernhard Ihrig[2], •Daniel Kruti[3], John A. Gracey[4], Michael M. Scherer[2], and Lukas Janssen[1] — [1]TU Dresden — [2]University of Cologne — [3]University of Cologne and Jülich Research Centre — [4]University of Liverpool

Two-dimensional spin-orbital magnets with strong exchange frustration have recently been predicted to realise a quantum critical point in the Gross-Neveu-SO(3) universality class. In contrast to previously known Gross-Neveu-type universality classes, this quantum critical point separates a Dirac semimetal and a long-range-ordered phase, in which the fermion spectrum is only partially gapped out. Here, we characterise the quantum critical behaviour of the Gross-Neveu-SO(3) universality class by employing three complementary field-theoretical techniques beyond their leading orders. We compute the correlation-length exponent ν, the order-parameter anomalous dimension η_ϕ, and the fermion anomalous dimension η_ψ using a three-loop 4-ϵ expansion, a second-order large-N expansion (with the fermion anomalous dimension obtained even at the third order), as well as a functional renormalisation group approach. The results from the different methods agree well with each other and provide a prime benchmark for future complementary calculations. Averaging over them, we obtain the estimates $1/\nu = 1.03(15)$, $\eta_\phi = 0.42(7)$, and $\eta_\psi = 0.180(10)$ for the physically relevant case of $N = 3$ flavours of two-component Dirac fermions in 2+1 space-time dimensions.

TT 23.4 Wed 15:45 H22

Spin excitations in the frustrated helimagnet FeP — •Aleksandr Sukhanov, Yuliia Tymoshenko, Anton Kulbakov, and Dmytro Inosov — Institut für Festkörper- und Materialphysik, Technische Universität Dresden, D-01069 Dresden

The metallic compound FeP belongs to the class of materials that feature a complex noncollinear spin order driven by the magnetic frustration. While its double-helix magnetic structure with a period $\lambda_s \approx 5c$, where c is the lattice constant, was previously well determined, the relevant spin-spin interactions that lead to that ground state remain unknown. By performing extensive inelastic neutron scattering measurements, we obtained the spin-excitation spectra in a large part of the momentum-energy space. The spectra show that the magnons are gapped with a gap energy of ~5 meV. Despite the 3D crystal structure, the magnon modes display strongly anisotropic dispersions, revealing quasi-one-dimensional character of the magnetic interactions in FeP. The physics of the material, however, is not determined by the dominating exchange, which is ferromagnetic. Instead, the weaker two-dimensional antiferromagnetic interactions between the rigid ferromagnetic spin chains drive the magnetic frustration. Using linear spin-wave theory, we were able to construct an effective Heisenberg Hamiltonian with an anisotropy term capable of reproducing the observed spectra. This enabled us to quantify the exchange interactions in FeP and determine the mechanism of its magnetic frustration.

TT 23.5 Wed 16:00 H22

NMR and magnetization studies of helical correlations within the stretched diamond lattice of $LiYbO_2$ — •S. Luther[1,2], S. Wilson[3], M. M. Bordelon[3], J. Wosnitza[1,2], M. Baenitz[4], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]University of California, Santa Barbara, USA — [4]MPI for Chemical Physics of Solids, Dresden, Germany

The Yb-based delafossite $LiYbO_2$ hosts a stretched diamond lattice. The resulting three-dimensional geometric frustration is in strong contrast to the recently reported 2D-type Yb-based triangular-lattice delafossites. Further, the combination of a strong spin-orbit coupling together with crystalline-electric-field effects leads to a pseudospin-1/2 ground state of the Yb^{3+} ions. A recent study of $LiYbO_2$ by means of specific heat and neutron powder diffraction established the formation of helical order with non-trivial phasing between the two interpenetrating Yb sublattices below 1.1 K [1]. In order to further explore the H-T phase diagram and magnetic correlations, we performed low-temperature magnetometry and ^{7}Li NMR of polycrystalline $LiYbO_2$. Our magnetometry and $1/T_1$ NMR data are fully consistent with the reported specific-heat results. The ^{7}Li NMR spectroscopy yields a monotonic and asymmetric spectral broadening towards low temperatures in the paramagnetic state. In the helical ordered state, a spontaneous and pronounced increase of the spectral width is observed, in agreement with the neutron-diffraction experiments.

[1] Bordelon *et al.*, Phys. Rev. B **103**, 014420 (2021)

TT 23.6 Wed 16:15 H22

Nonlinear stress-strain relation of $PdCrO_2$ — •Nina Stilkerich[1,2], Hilary Noad[1], Seunghyun Khim[1], Andrew Mackenzie[1,3], and Clifford Hicks[1,4] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 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 delafossite with an antiferromagnetic triangular lattice and a Neel temperature of 38 K. It has a double-q magnetic structure, in which the direction of spin rotation alternates from layer to layer. Under uniaxial stress, $PdCrO_2$ undergoes a transition from this double- to a single-q structure. Here, we will show stress-strain data on $PdCrO_2$, collected using a piezoelectric-driven strain cell that allows simultaneous measurement of uniaxial stress and strain. We will show that the change in lattice constant across this magnetic transition is quite large and that the transition evolves in a nontrivial way as temperature is raised.

15 min. break

TT 23.7 Wed 16:45 H22

Magneto-thermodynamics of the J_1-J_2 Heisenberg antifer-

romagnet on the square lattice — •Andreas Honecker[1], Johannes Richter[2,3], Jürgen Schnack[4], Alexander Wietek[3], and Mike E. Zhitomirksy[5] — [1]LPTM, CY Cergy Paris Université, France — [2]Institut für Physik, Universität Magdeburg, Germany — [3]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [4]Fakultät für Physik, Universität Bielefeld, Germany — [5]Université Grenoble Alpes, CEA, IRIG, PHELIQS, France

We investigate the finite-temperature properties of the J_1-J_2 Heisenberg antiferromagnet on the square lattice in the presence of an external magnetic field. We focus on the highly frustrated regime around $J_2 \approx J_1/2$. The H-T phase diagram is investigated with particular emphasis on the finite-temperature transition into the "up-up-up-down" state that is stabilized by thermal and quantum fluctuations and manifests itself as a plateau at one half of the saturation magnetization in the quantum case. Furthermore, we discuss the enhanced magnetocaloric effect associated to the ground-state degeneracy that arises at the saturation field for $J_2 = J_1/2$. Computations for the spin-1/2 system are carried out using finite-temperature Lanczos and quantum typicality approaches.

TT 23.8 Wed 17:00 H22

One- and two-particle dynamics of the J_1-J_2-Heisenberg bilayer — •Erik Wagner and Wolfram Brenig — TU Braunschweig, Braunschweig, Germany

The antiferromagnetic J_1-J_2 Heisenberg-model on the square lattice is one of the pillars of frustrated quantum magnetism, with Néel- and collinearly ordered ground states competing for large and small J_1/J_2, and with a quantum disordered phase of still unsettled nature in between. Probing fingerprints of such phases by approaching them out of a well controlled dimer phase is one of the rationals for studying bilayer versions of frustrated spin models. Here, and starting from the limit of decoupled dimers, we use the perturbative Continuous Unitary Transformation (pCUT), based on the flow equation method, to perform series expansion in order to analyze the spectrum of the square lattice J_1-J_2-Heisenberg bilayer up to the two-triplon excitations. Evaluating the ground state energy and the one-particle dispersion up to 7th order in $J_{1,2}$ as well as the two-particle interactions and spectrum up to 5th order, we find emerging (anti-)bound two-particle states, which can be classified by total spin and real-space symmetry, consistent with results found for the J_1-only bilayer on the square lattice [1]. We analyze the phase boundary of the dimer phase with respect to one- and two-particle excitations and find reasonable agreement with recent coupled-cluster calculations [2], while also uncovering prospects for an additional phase introduced by two-particle boundstate condensation.

[1] A. Collins, C.J. Hamer, PRB 78, 054419 (2008)
[2] R.F. Bishop et al., PRB 100, 024401 (2019)

TT 23.9 Wed 17:15 H22

Entanglement measures of a frustrated spin-1/2 Heisenberg octahedral chain within the localized-magnon approach — •Olesia Krupnitska — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany — Institute for Condensed Matter Physics, NASU, Svientsitskii Str. 1, 79011 Lviv, Ukraine

The localized-magnon theory [1] is a powerful tool for the rigorous determination of the ground state and detailed study of the thermodynamic properties of a special class of frustrated quantum Heisenberg antiferromagnets at high magnetic fields and low temperatures. We study different measures of two-spin entanglement [2] between the nearest- and between next-nearest-neighbor spins on the square of the spin-1/2 octahedral Heisenberg chain. It was shown that the localized-magnon theory can be modified for simpler calculation of concurrence [3], which may serve as a measure of the bipartite entanglement of the octahedral chain. Furthermore, we calculate the entanglement of formation and the negativity [4] within the localized-magnon concept. We demonstrate that localized-magnon theory can be straightforwardly adapted in order to calculate the respective entanglement measures for a wide class of flat-band quantum Heisenberg antiferromagnets.

[1] J. Schulenburg et al., Phys. Rev. Lett. **88**, 167207 (2002).
[2] L. Amico et al., Rev. Mod. Phys. **80**, 517 (2008).
[3] J. Strečka, O. Krupnitska and J. Richter, EPL, **132** 30004 (2020).
[4] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996).

TT 23.10 Wed 17:30 H22

Interacting magnons in the easy-axis square-lattice XXZ-model and extensions towards ring exchange — •Dag-Björn Hering[1], Matthias R. Walther[2], Kai P. Schmidt[2], and Götz S. Uhrig[1] — [1]Technische Universität Dortmund, Department of Physics, Condensed Matter Theory, Otto-Hahn-Str. 4, 44227 Dortmund — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Theoretische Physik I, Staudtstraße 7, 91058 Erlangen

The method of non-perturbative continuous similarity transformations (CST) in momentum space captures the physics of the isotropic spin 1/2 antiferromagnetic Heisenberg model on the square lattice (IHM) quantitatively [1-2]. We extend these studies to single- and two-particle properties of models related to the IHM. We start with easy-axis square-lattice XXZ-model as simplemost extension of the IHM. Here, we present and discuss the CST results for the gap [3], the roton mode [4] and the bound-states [3] between the Ising limit to isotropic point in comparison to other methods. In addition, we outline further applications of the CST to models with ring-exchange [5] relevant for cuprates and the J-Q Model as an variant of ring-exchange without frustration [6].

[1] M. Powalski et al., Phys. Rev. Lett. 115, 207202 (2015)
[2] M. Powalski et al., SciPost Phys. 4, 001 (2018)
[3] S. Dusuel et al., Phys. Rev. B 81, 064412 (2010)
[4] R. Verresen et al., Phys. Rev. B 98, 155102 (2018)
[5] K. Majumdar et al., Phys. Rev. B 85, 144420 (2012)
[6] A. W. Sandvik Phys. Rev. Lett. 98, 227202 (2007)

TT 23.11 Wed 17:45 H22

Towards analyzing phase-transitions with continuous similarity transformation: Easy-axis square-lattice XXZ and J_1-J_2 models — •Matthias R. Walther[1], Dag-Björn Hering[2], Götz S. Uhrig[2], and Kai P. Schmidt[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Theoretische Physik I, Staudtstraße 7, 91058 Erlangen — [2]Technische Universität Dortmund, Department of Physics, Condensed Matter Theory, Otto-Hahn-Str. 4, 44227 Dortmund

The method of non-perturbative continuous similarity transformations (CST) in momentum space captures the physics of the isotropic spin 1/2 antiferromagnetic Heisenberg model on the square lattice (IHM) quantitatively [1,2]. We discuss the potential of the CST to study critical behavior. To this end, the easy-axis square-lattice XXZ-model serves as a straight-forward extension of the IHM with a gapped phase away from the isotropic point. Its critical behavior is described by an established mean-field theory [3]. The CST is able to capture this criticality quantitatively. For further insights on the general capability of the CST for spin models we extend the study towards the frustrated square-lattice spin 1/2 antiferromagnetic J_1-J_2 model and analyze the breakdown of the magnetically ordered quantum phases and their gapless spin wave excitations [4,5].

[1] M. Powalski et al., Rev. Lett. 115, 207202 (2015)
[2] M. Powalski et al., SciPost Phys. 4, 001 (2018)
[3] W. Zheng et al., Phys. Rev. B 71, 184440 (2005)
[4] Götz S. Uhrig et al., Phys. Rev. B 79, 092416 (2009)
[5] R. R. P. Singh et al., Phys. Rev. Lett. 91, 017201 (2003)

TT 23.12 Wed 18:00 H22

"Stripe-yz" magnetic order in $KCeS_2$ — •Anton Kulbakov[1,2], Stanislav Avdoshenko[3], Inés Puente-Orench[4,5], Jacques Ollivier[5], Mahmoud Deeb[1], Mathias Doerr[1], Philipp Schlender[6], Thomas Doert[6], and Dmytro Inosov[1,2] — [1]IFMP, TU Dresden, Germany — [2]Würzburg-Dresden ct.qmat, TUD, Dresden, Germany — [3]IFW, Dresden, Germany — [4]INMA, Zaragoza, Spain — [5]ILL, Grenoble, France — [6]Fakultät für Chemie und Lebensmittelchemie, TU Dresden, Germany

We have solved the magnetic structure for the antiferromagnetic state below $T_N = 400$ mK, which was recently revealed in the effective spin-1/2 triangular-lattice antiferromagnet $KCeS_2$. It represents the so-called "stripe-yz" type of antiferromagnetic order with spins lying approximately in the triangular-lattice planes orthogonal to the nearest-neighbor Ce—Ce bonds, possibly with a small out-of-plane canting of the magnetic moments. The thermal expansion remains very small below 120 K, which we confirmed for the c lattice constant using capacitive dilatometry. Our experimental results also indicate that cerium oxysulphide, Ce_2O_2S, which was present in our sample as a minority phase, does not order magnetically down to 20 mK and may therefore represent a promising spin-liquid candidate deserving a separate study. For details, see [1]. Neutron time-of-flight spectroscopy of low-energy excitations in the ordered state of $KCeS_2$ reveals an unusual spin-wave band with an intensity maximum at $\mathbf{Q} = 0$, unlike in $KCeO_2$ and $KYbSe_2$.

[1] J. Phys.: Condens. Matter **33**, 425802 (2021)

TT 23.13 Wed 18:15 H22

Quantum Skyrmion lattices in Heisenberg ferromagnets — •Andreas Haller, Solofo Groenendijk, Alireza Habibi, Andreas Michels, and Thomas L. Schmidt — Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

Skyrmions are topological magnetic textures that can arise in noncentrosymmetric ferromagnetic materials. In most systems experimentally investigated to date, skyrmions emerge as classical objects. However, the discovery of skyrmions with nanometer length scales has sparked interest in their quantum properties. In this talk, we present the results of our matrix product state simulations of the ground states of two-dimensional spin-1/2 Heisenberg lattices with Dzyaloshinskii-Moriya interactions. We discovered a broad region in the zero-temperature phase diagram which hosts quantum skyrmion lattices. The quantum skyrmion lattice phase can be detected experimentally in the magnetization profile via local magnetic polarization measurements as well as in the spin structure factor measurable via neutron scattering experiments. Finally, we show the real-space polarization profile of individual quantum skyrmions and show that it is a non-classical state featuring entanglement between quasiparticle and environment mainly localized near the boundary spins of the skyrmion.