MA 21: Frustrated Magnets I

Time: Wednesday 9:30–12:45 Location: H18

MA 21.1 Wed 9:30 H18

Ab-initio exploration of complex magnetism of frustrated Mn and Cr films on hexagonal metallic surfaces — •Selcuk Sözeri[1,2] and Samir Lounis[2,1] — [1]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

We employ ab initio first-principles simulations to explore the complex magnetic behavior in antiferromagnetic (AFM) systems. Specifically, we investigate Mn films on an Ag(111) substrate, where spin-polarized STM experiments established Néel order as the ground state for a single Mn layer [1,2] in contrast to previous predictions. Our focus extends to the interplay of Heisenberg exchange interactions, leading to magnetic frustration, and higher-order magnetic interactions when increasing the thickness of Mn films, which can host complex three-dimensional AFM spin-textures. Additionally, we examine the magnetic properties of multiple AFM Cr layers deposited on a PdFe bilayer supported by an fcc Ir(111) substrate. Instead of being in a Néel state, a single Cr layer prefers a row-wise AFM state, which hosts single and catenated intrinsic AFM skyrmions [3]. For thicker Cr films, we monitor the emergence of new topological magnetic objects.

– Project funded by DFG (SPP 2137: LO 1659/8-1).

– [1] Gao, et al., PRL 101, 267205 (2008); [2] Sözeri et al., submitted (2024); [3] Aldarawsheh et al., Nat. Commun.13, 7369 (2022); Front. Physics. 11, 335 (2023).

MA 21.2 Wed 9:45 H18

Dilatometry studies on the spin supersolid candidate materials $K_2Co(SeO_3)_2$ and $Rb_2Co(SeO_3)_2$ — •Erik Walendy[1], Kwangwoo Shin[2], Jae-Ho Chung[2], Kwang-Yong Choi[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Department of Physics, Korea University, Seoul 02841, Korea

The layered triangular lattice material $K_2Co(SeO_3)_2$ has recently attracted attention due to the presence of a high-field spin supersolid phase between 18 and 21 T, at 2 K [1]. We report high-resolution capacitance dilatometric studies on single crystals of $K_2Co(SeO_3)_2$ and $Rb_2Co(SeO_3)_2$. Pronounced anomalies in thermal expansion and magnetostriction measurements at the phase boundaries imply significant magnetoelastic coupling. We obtain the uniaxial strain dependencies of the field-induced phases and construct the magneto-elastic phase diagrams.

[1] T. Chen et al. arXiv:2402.15869 (2024).

MA 21.3 Wed 10:00 H18

NMR Study of the $S = 1/2$ 1D Heisenberg Antiferromagnetic Chain $Cu(C_6H_8N_2)ClBr$ — •Marlis Schuller[5], Monika Jawale[1], Avinash Mahajan[1], Sanjay Bachhar[1], Saikat Nandi[1], Rahul Kumar[2], Athinarayanan Sundaresan[2], John Wilkinson[3], Rabindranath Bag[4], Sara Haravifard[4], Norbert Büttgen[5], Thomas Gimpel[5], and István Kézsmárki[5] — [1]Department of Physics, IIT Bombay, IN — [2]CPMU, JNCASR, IN — [3]ISIS Facility, STFC Rutherford Appleton Laboratory, GB — [4]Department of Physics, Duke University, US — [5]EPV, Institute of Physics, University of Augsburg, DE

$Cu(C_6H_8N_2)ClBr$ is a possible candidate for realising the frustration-induced quantum spin-liquid phase, as proposed in a recent theoretical study by Uematsu *et al.* (JPSJ **90**, 124703 (2021)) on the random-bond $S = 1/2$ Heisenberg antiferromagnet on the zigzag chain. Based on μSR and bulk susceptibility data, it does not display any long-range order down to 88 mK. Mixing chlorine and bromine may generate randomness in the nearest-neighbour exchange necessary to satisfy the criteria from the aforementioned proposal. We investigated this compound by ^{1}H-NMR, and determined the spin-lattice relaxation rate $1/T_1(T)$ to probe low-energy excitations. Our study revealed a discontinuity in the relaxation rate at a characteristic temperature of approximately 2.5 K, where anomalies were observed in the specific heat and μSR experiments. These experimental results imply the emergence of a dimerised ground state.

MA 21.4 Wed 10:15 H18

Geometric design of frustrated magnetic textures in ferrotoroidal spin chains — •Oleksandr V. Pylypovskyi[1], Enrico Di Benedetto[2], Carmine Ortix[3], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany — [2]Università degli Studi di Palermo, 90123 Palermo, Italy — [3]Università di Salerno, IT-84084 Fisciano (SA), Italy

Design of geometric shapes in magnetic nanosystems provides a possibility to tune their magnetic responses [1] and even enable multiferroicity by a finite geometry-driven toroidal moment [2]. Here, we consider the effects of ring-like geometries with a constant torsion on properties of 3D ferro- (FM) and antiferromagnetic (AFM) spin chains. Their magnetic state is primarily determined by the knots in geometry with a high curvature, which corresponds to a localized geometry-driven Dzyaloshinskii–Moriya interaction (DMI). This DMI favors the twist of the order parameter at the knot. For the AFM chains with even and odd number of spins, the number of knots in their geometry allows designing the ground-state magnetic texture characteristic either for the spin system with or without geometric frustration. While the FM chains with the easy tangential axis of magnetization host a large toroidal moment for the whole sample, AFM hard-axis chains split into toroidal domains by geometric knots. To conclude, the localized geometry-driven DMI offers a possibility to design frustrated magnetic textures in spin chains.

[1] D. Makarov et al., Adv. Mater. 34, 2101758 (2022). [2] C. Ortix, J. van den Brink, Phys. Rev. Research, 5, L022063 (2023).

MA 21.5 Wed 10:30 H18

High-temperature expansion of dynamical spin correlator: Dyn-HTE — •Ruben Burkard[1], Benedikt Schneider[2,3], and Björn Sbierski[1] — [1]Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [2]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Currently, there is a scarcity of theoretical methods to calculate dynamical correlation functions at finite temperatures in frustrated spin systems. To address this challenge, we extend the well-established method of high-temperature expansion to the dynamical two-point Matsubara Green's function, which we calculate to high order in perturbation theory. We consider Heisenberg models with one coupling constant J, arbitrary spin length, and without external magnetic field. We use resummation techniques to extrapolate our results to temperatures down to about $T \approx 0.2J$. Our method also gives an analytical expression for the frequency dependence, enabling analytical continuation to real frequencies. Using the dynamical information of the Matsubara correlator, we aim to study spin-liquid phases with this approach in the future.

MA 21.6 Wed 10:45 H18

Pseudo-Majorana Functional Renormalization for Frustrated XXZ-Z Spin-1/2 Models — Ruben Burkard[1], Benedikt Schneider[2], and •Björn Sbierski[1] — [1]Universität Tübingen — [2]LMU München

The numerical study of high-dimensional frustrated quantum magnets remains a challenging problem. Here we present an extension of the pseudo-Majorana functional renormalization group to spin-1/2 XXZ type Hamiltonians with field or magnetization along spin-Z direction at finite temperature. We consider a U(1) symmetry-adapted fermionic spin representation and derive the diagrammatic framework and its renormalization group flow equations. We discuss benchmark results and application to two anti-ferromagnetic triangular lattice materials recently studied in experiments with applied magnetic fields: First, we numerically reproduce the magnetization data measured for CeMgAl11O19 confirming model parameters previously estimated from inelastic neutron spectrum in high fields. Second, we showcase the accuracy of our method by studying the thermal phase transition into the spin solid up-up-down phase of Na2BaCo(PO4)2 in good agreement with experiment.

15 min. break

MA 21.7 Wed 11:15 H18

NMR study of the field-induced magnetic states in Cu-based mineral $Cu_2(OH)_3NO_3$ — •Yoshihiko Ihara[1], Issei Niwata[1], Aswathi M. Chakkingal[2], Dmytro Inosov[2], and Darren Peets[2] — [1]Hokkaido University, Sapporo, Japan — [2]TU Dresden, Dresden, Germany

Magnetic ground states are stabilized at low temperature by minimizing the energy costs for magnetic moments interacting with each other. When the interactions compete by geometrical frustration in the case of a non-bipartite lattice or by the bond-dependent sign of interactions, the magnetic ground state cannot be easily selected and the perturbation by external fields can modify the ground state introducing a nontrivial magnetic state with intriguing properties. Here, we focus on the Cu-based mineral rouaite, $Cu_2(OH)_3NO_3$, in which $S = 1/2$ Cu^{2+} spins construct both ferromagnetic (FM) and antiferromagnetic (AFM) chains in a unit cell. Competing FM and AFM interactions result in complicated field-temperature phase diagram with at least three different magnetic states. We study the magnetic structure and the low-energy magnetic excitations by measuring the NMR spectra and the nuclear spin-lattice relaxation rate. The low-field magnetic structure is identified and compared with the results of neutron diffraction measurements. We will also discuss the external magnetic field effect on the magnetic ground state from the results of NMR measurements at higher magnetic fields.

MA 21.8 Wed 11:30 H18

Magnetic Properties of the Frustrated Cu-based Quantum Magnets Posnjakite, Kobyashevite, and Ktenasite — Kaushick K. Parui[1], Anton A. Kulbakov[1], Roman Gumeniuk[2], Sergey Granovsky[1], Dmytro S. Inosov[1], and •Darren C. Peets[1] — [1]IFMP, TU Dresden, Germany — [2]IEP, TU Bergakademie Freiberg, Germany

Posnjakite, kobyashevite, and ktenasite are copper hydroxide sulphates in which the magnetic copper sites are arranged in distorted-triangular planes. Such a magnetic sublattice is expected to lead to strong geometric frustration, which can produce exotic magnetic order. We report the synthesis of all three materials and the results of our investigations into their low temperature magnetic properties by magnetization, specific heat, and diffraction. All three compounds indeed exhibit low magnetic transition temperatures with high frustration factors, confirming that frustration plays a key role in selecting their magnetic ground states.

MA 21.9 Wed 11:45 H18

The role of quantum fluctuations in rare-earth pyrochlore oxides — •Lasse Gresista[1], Daniel Lozano-Gómez[2], Simon Trebst[1], and Yasir Iqbal[3] — [1]Institute for Theoretical Physics, University of Cologne — [2]Institut fur Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universitat Dresden — [3]Department of Physics and Quantum Center for Diamond and Emergent Materials (QuCenDiEM), Indian Institute of Technology Madras, Chennai, India

Rare-earth pyrochlore oxides provide a rich platform for exploring exotic magnetic phenomena, ranging from the highly degenerate spin-ice states governed by emergent gauge theories in $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$, to order-by-disorder effects in $Er_2Ti_2O_7$, multi-phase magnetism in $Yb_2Ti_2O_7$, and the ongoing quest to realize a quantum spin liquid state in experiment. Many of these materials are well described by localized spin-$\frac{1}{2}$ moments on a pyrochlore lattice coupled via anisotropic interactions. While the classical limit of this model has been extensively studied, a full quantum mechanical treatment remains challenging. In this work, we investigate the general spin-$\frac{1}{2}$ Hamiltonian using a pseudo-fermion functional renormalization group approach, which incorporates quantum fluctuations beyond mean-field theory. Our results reveal a significant shift in phase boundaries compared to the classical model, alongside the emergence of disordered regions without conventional magnetic order. This highlights the importance of quantum fluctuations when interpreting experimental observations in pyrochlore magnets.

MA 21.10 Wed 12:00 H18

Dynamical response of the Kitaev quantum spin liquid in the $KJ\Gamma$-model under external magnetic field — •Peng Rao[1], Roderich Moessner[2], and Johannes Knolle[1,3,4] — [1]Physics Department, Technical University of Munich, TUM School of Natural Sciences, 85748 Garching, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [4]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

We study the dynamical structure factor of the Kitaev quantum spin liquid (KQSL) generally, i.e. away from the solvable Kitaev limit, in the $KJ\Gamma$-model with external magnetic field. Using Majorana mean field theory, we compute spin susceptibility by including Majorana interactions in the random phase approximation (RPA). At zero field for the pure Kitaev model, RPA reproduces qualitatively spin susceptibility in the adiabatic approximation, which is close to the exact result. Small non -Kitaev couplings J and Γ induce sharp low-energy magnon modes as Majorana bound states. Larger couplings or finite field generally tend to weaken the KQSL and cause the sharp modes to condense, whence the system becomes magnetically ordered. However in specific paramter regimes, magnetic field may destroy the zero-field magnetic order and stabilize KQSL at intermediate field values, thus exemplifying the proposed 'field-induced KQSL'.

MA 21.11 Wed 12:15 H18

Short-range spin correlations in the 3D face-centred frustrated spin-$\frac{5}{2}$ system $MnSn(OH)_6$ — •Kaushick K. Parui[1], Anton A. Kulbakov[1], Ellen Häussler[2], Nikolai S. Pavlovskii[1], Roman Gumeniuk[3], Thomas Doert[2], Maxim Avdeev[4], Dmytro S. Inosov[1], and Darren C. Peets[1] — [1]IFMP, TU Dresden, Germany — [2]AC II, TU Dresden, Germany — [3]IEP, TU Bergakademie Freiberg, Germany — [4]ANSTO, Australia

Manganese tin hydroxide, $MnSn(OH)_6$, is an A-site-vacant double perovskite with magnetic Mn^{2+} ions on a face-centred sublattice, creating frustration that may lead to exotic magnetism. Combined x-ray and neutron diffraction data analysis reveals tetragonal $P4_2/n$ symmetry with precise H/D positions. Despite dominant antiferromagnetic interactions among Mn^{2+} moments, evidenced by a negative Curie-Weiss temperature, the lack of a sharp thermodynamic transition down to 350 mK implies the absence of long-range magnetic order. This suppression of the magnetic order hints towards a large frustration factor >10. Low-temperature neutron diffraction performed at 20 mK shows the absence of sharp magnetic Bragg peaks but reveals broad diffuse peaks, indicating 3D antiferromagnetic short-range interactions with a correlation length of roughly three unit cells.

MA 21.12 Wed 12:30 H18

Understanding the Hamiltonian of α-$RuCl_3$ through Nonlinear Spin-Wave Analysis — •Jonas Habel[1,2], Roderich Moessner[3] und Johannes Knolle[1,2,4] — [1]Technical University of Munich, Germany — [2]Munich Center for Quantum Science and Technology, Germany — [3]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [4]Blackett Laboratory London, UK

The precise values of the magnetic exchange couplings in α-$RuCl_3$ are of significant interest to understand the proposed Kitaev spin-liquid phase. A common method for extracting them involves fully field-polarizing the magnetic moments, performing an inelastic neutron scattering (INS) experiment, and fitting a non-interacting (linear) spin-wave theory to the data. However, due to magnetic frustration, magnon many-body interactions are strong in α-$RuCl_3$ and cannot be neglected, even at high fields. We present a procedure for fitting an interacting (nonlinear) spin-wave theory to INS data, explicitly accounting for these many-body interactions. This reveals a significant renormalization of the exchange couplings compared to linear spin-wave estimates.