TT 26: Correlated Magnetism – Frustrated Systems

Time: Tuesday 9:30–12:15 Location: HSZ/0103

TT 26.1 Tue 9:30 HSZ/0103

Finite-temperature Lanczos approach to frustrated quantum spin systems — •Andreas Honecker[1], Malo Rouxel[1], and Katarína Karľová[2] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS, CY Cergy Paris Université, France — [2]Department of Theoretical Physics and Astrophysics, P.J. Šafárik University, Košice, Slovakia

The finite-temperature Lanczos method or its quantum typicality variants are a method of choice for computing thermodynamic properties of frustrated quantum spin systems, in particular in two dimensions. Here we show that quasi-exact results can be obtained with moderate numerical effort for systems with $N \leq 40$ spins $1/2$, even if the method involves Monte Carlo sampling. We illustrate the approach on the diamond-decorated square and honeycomb lattices. These models not only distinguish themselves by the presence of local conservation laws, but also offer a rich phase diagram, including phases with macroscopic ground-state degeneracy. We comment in particular on the resulting enhanced magnetocaloric effect [1].

[1] K. Karľová, A. Honecker, N. Çaçi, S. Wessel, J. Strečka, T. Verkholyak, Phys. Rev. B **110**, 214429 (2024).

TT 26.2 Tue 9:45 HSZ/0103

Quantum annealing for lattice models with long-range interactions — •Jan Alexander Koziol and Kai Phillip Schmidt — Department of Physics, Staudtstraße 7, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), D-91058 Erlangen, Germany

We use superconducting qubit quantum annealing devices to determine the ground state in the thermodynamic limit of Ising models with algebraically decaying long-range interactions. This is enabled by a unit-cell-based optimization scheme, in which the finite optimizations on each unit cell are performed using commercial quantum annealing hardware. To demonstrate the capabilities of the approach, we choose three exemplary problems relevant for other quantum simulation platforms and material science: (i) the calculation of devil's staircases of magnetization plateaux of the long-range Ising model in a longitudinal field on the triangular lattice, motivated by atomic and molecular quantum simulators; (ii) the evaluation of the ground state of the same model on the Kagomé lattice in the absence of a field, motivated by artificial spin ice; (iii) the study of models with modified few-nearest-neighbor interactions relevant for Ising compounds with potential long-range interactions. The approach discussed in this work provides a useful and realistic application of existing quantum annealing technology, applicable across many research areas in which lattice problems with resummable long-range interactions are relevant.

TT 26.3 Tue 10:00 HSZ/0103

Nature of intersite exchange interactions in Ce triangular-lattice delafossites — •Leonid Pourovskii — CPHT, CNRS, Ecole polytechnique, IP Paris, 91120 Palaiseau, France — Collège de France, Université PSL, 75005 Paris, France

Anisotropic intersite exchange interactions (IEI) in frustrated rare-earth magnets are difficult to assess both theoretically and experimentally. We propose an ab initio force-theorem framework combining the quasi-atomic Hubbard-I approach to $4f$ correlations with a static mean-field treatment of the on-site intershell Coulomb interaction between rare-earth $4f$ and $5d$ states to simultaneously capture both $4f$ superexchange and $5d$-mediated indirect exchange. Applying it to a set of Ce delafossites – the selenide $CsCeSe_2$, sulfide $KCeS_2$, and oxide $RbCeO_2$ – we find a remarkable qualitative evolution of IEI. While the superexchange is found to dominate over the indirect exchange in the oxide, the situation is reversed in the selenide. Both coupling mechanisms are found to contribute comparably in the sulfide. The calculated IEI place $CsCeSe_2$ and $KCeS_2$ in the yz-stripe region of the published spin-1/2 triangular-lattice model phase diagram, in agreement with experiment, while those for $RbCeO_2$ correspond to the 120° antiferromagnetic order. The magnetic excitation spectra of $CsCeSe_2$ and $KCeS_2$ evaluated from the calculated spin Hamiltonains are in good qualitative and quantitative agreement with experimental data.

TT 26.4 Tue 10:15 HSZ/0103

Quantum Monte Carlo study of the Su-Schrieffer-Heeger model on a triangular lattice — •Disha Hou[1], Anika Götz[1], Jadson Silva[2], Natanael Costa[2], and Fakher Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Universitat Würzburg, Würzburg, Germany — [2]Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil

We study the half-filled bond Su-Schrieffer-Heeger (SSH) model on the triangular lattice using sign-problem-free auxiliary-field quantum Monte Carlo methods. By varying the hopping matrix element, we interpolate between the assisted hopping limit — characterized by an emergent local $\mathbb{Z}_2$ symmetry and phases in which the hopping is weakly modulated by phonons. In addition to a s-wave superconducting state and a staggered valence-bond solid state, we observe an emergent flux phase which, in the absence of fluctuations, would exhibit a Dirac dispersion. We find that this phase is gapped and does not appear to break any ultraviolet symmetries of the model, leading us to tentatively identify it as a gapped Z_2 quantum spin liquid phase.

TT 26.5 Tue 10:30 HSZ/0103

Exact nematic and mixed magnetic phases driven by competing orders on the pyrochlore lattice — •Niccolò Francini, Lukas Schmidt, Lukas Janssen, and Daniel Lozano-Gómez — Institut für Theoretische Physik und Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany

Pyrochlore magnets are a paradigmatic example of three-dimensional frustrated systems and provide an excellent platform for studying a variety of exotic many-body phenomena. In recent years, increasing attention has been devoted to bilinear spin models on this lattice, where multiple magnetic phases can be degenerate in energy, often stabilizing unconventional magnetic states. In this work, we focus on one such model, parametrized by the interaction coupling $J_{z\pm}$, which defines a line in parameter space corresponding to the phase boundary between three distinct magnetic phases. Using a combination of analytical and numerical methods, we show that this model exhibits an order-by-disorder mechanism at low temperatures, giving rise to a *mixed* magnetic phase. This represents the first realization of a $\mathbf{q} = 0$ long-range-ordered phase in a pyrochlore magnet characterized by two distinct order parameters, which we denote as the $A_2 \oplus \psi_2$ phase. Furthermore, at $J_{z\pm} = 1/\sqrt{2}$, the model acquires a subextensive number of discrete symmetries, which preclude the stabilization of conventional long-range order and instead lead to the emergence of a novel nematic phase. We characterize this nematic phase, describe how its ground-state configurations are constructed, and analyze its stability at higher temperatures and under small deviations from $J_{z\pm} = 1/\sqrt{2}$.

TT 26.6 Tue 10:45 HSZ/0103

From Open-Shell Nanographenes to Quantum Spin Chains: Controllable Spins in Carbon Ladders — •Andoni Agirre[1,2], Thomas Frederiksen[1,3], Géza Giedke[1,3], and Tobias Grass[1,3] — [1]Donostia International Physics Center (DIPC), Manuel Lardizabal Pasealekua 4, 20018 Donostia, Basque Country — [2]Department of PMAS: Physics, Chemistry and Technology, University of the Basque Country (UPV/EHU), Manuel Lardizabal Pasealekua 3, 20018 Donostia, Basque Country — [3]IKERBASQUE, Basque Foundation for Science, Euskadi Plaza 5, 48009 Bilbao, Basque Country

The low-energy electronic structure of nanographenes with open-shell configurations can be faithfully represented by effective quantum spin models, providing a promising route toward carbon-based quantum simulators. Here we demonstrate this correspondence for an oligo-indenoindene molecule, composed of alternating pentagon-hexagon rings and theoretically mapped to a frustrated Fermi-Hubbard ladder. We show that a spin-1/2 Heisenberg chain consisting of only one spin per pentagon and featuring nearest- and next-nearest-neighbor couplings, quantitatively reproduces the molecular excitation spectrum and entanglement structure obtained from matrix-product-state calculations. By systematically identifying the effective spins with delocalized fermionic modes across the molecular backbone, we achieve near-quantitative agreement in both static and dynamical magnetic properties. Our results establish them as experimentally realizable platforms for exploring frustrated magnetism and correlated spin dynamics in purely carbon-based materials.

15 min. break

TT 26.7 Tue 11:15 HSZ/0103

Single crystal growth and study of the spin gap system Cu_3WO_6 — •Annarose Jose Palliyan[1,2], Nazmul Islam[2], Cintli Aguilar-Maldonado[2], Ralf Feyerherm[2], Andrey Malyuk[3], Sabine Wurmehl[3], and Bella Lake[2,1] — [1]Technische Universität Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Leibniz Institute for Solid State and Materials Research Dresden, Germany

Frustration in magnetic materials is an important phenomena leading to exotic quantum states due to the presence of the competing interactions in those materials. From this point of view, cuprates are interesting because of the possibility of having multiple correlations and interactions resulting in unusual correlated phases[1]. Copper tungstate, Cu_3WO_6, is one such compound where Cu^{2+} (S=1/2) occupies the triangular bipyramidal sites. This cubic system (Pa-3) hosts a unique magnetic lattice consisting of coupled hexagons and equilateral triangles of Cu^{2+} giving rise to multiple exchange interactions. In order to study the magnetic behavior and solve the magnetic Hamiltonian of this material, we have grown the first single crystals of Cu_3WO_6 by several different growth techniques and the high crystalline quality of these crystals has been confirmed. We have also studied the thermodynamic properties on these crystals down to low temperatures and our results confirm the reported singlet ground state with a spin gap of about 130K which suggests a dominant hexagonal interaction[2].

[1] Y. Fudamoto et al., Phy. Rev B 65, 174428 (2002)
[2] M. Hase et al., Phys. B: Condens. Matter 215, 325 (1995)

TT 26.8 Tue 11:30 HSZ/0103

Magnetic frustration and field-induced transitions in the octahedral lattice iridate Ho_3IrO_6 — •Abanoub Hanna[1], Cintli Aguilar Maldonado[1], Ralf Feyerherm[1], A.T. M. Nazmul Islam[1], and Bella Lake[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Platz 1, D-14109 Berlin, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Germany

Ho_3IrO_6 is a new octahedral lattice compound in which holmium ions form a distorted network of corner sharing octahedra, providing a clean platform to study frustration in rare earth iridates. X ray and neutron powder diffraction confirm a single phase cubic Ia-3 structure with ordered Ho and Ir sites and no detectable impurities, so the magnetic behaviour can be interpreted without structural complications. Low temperature magnetometry shows a sharp transition near 1 kelvin with strong field dependence, and Curie Weiss analysis indicates antiferromagnetic interactions and a large frustration parameter, pointing to competing exchanges on the octahedral lattice. AC susceptibility, nonlinear magnetization curves and field dependent anomalies reveal a genuine thermodynamic transition and metamagnetic steps, while heat capacity data are consistent with a low lying triplet ground state and an additional Schottky like feature around 5 K.

TT 26.9 Tue 11:45 HSZ/0103

Crystal growth, electronic and magnetic Properties of Mn_3Al_9Si — •Ashiwini Balodhi[1], Min Gyu Kim[2], Andreas Kreyssig[1], and Anna E. Böhmer[1] — [1]Experimental Physics IV, Ruhr-University Bochum, Bochum, Germany — [2]University of Wisconsin-Milwaukee, Milwaukee, USA

The Mn-based intermetallic compound Mn_3Al_9Si crystallizes in a hexagonal structure in which the Mn ions form a well-separated triangular network, giving rise to unusual transport and thermodynamic behavior. We have synthesized high-quality single crystals of Mn_3Al_9Si and performed magnetic, transport and heat-capacity measurements. The magnetic susceptibility exhibits isotropic behavior with no evidence of long-range magnetic ordering down to 1.8 K. Low-temperature resistivity measurements reveal a negative magnetoresistance. We further present the critical scaling behavior in applied magnetic fields, in both magnetization and heat-capacity.

We acknowledge funding from the European Research Council through Project 101040811, Distort-to-Grasp.

TT 26.10 Tue 12:00 HSZ/0103

Synthesis and characterization of $Mn_3Al_2Si_3O_{12}$ single crystal — •Marwa Abouelela[1,2], ATM Nazmul Islam[2], Ralf Feyerherm[2], and Bella Lake[1,2] — [1]Institut für Festkörperphysik, Technische Universität, Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Geometric magnetic frustration, typically found in materials with triangular and tetrahedral motifs, has attracted significant interest in recent research [1]. The garnet $Mn_3Al_2Si_3O_{12}$ exhibits geometrical frustration, where magnetic Mn^{2+} ($3d^5$) ions that have spin-5/2 form hyper-Kagome structure which is three-dimensional network of corner-sharing triangles [2]. In this study, we synthesized the first single crystals of $Mn_3Al_2Si_3O_{12}$ grown by the optical floating-zone technique. X-ray and neutron diffraction confirmed the garnet space group $Ia\bar{3}d$. Temperature-dependent magnetic susceptibility measurements reveal antiferromagnetic ordering of the Mn^{2+} ions below $T_N = 6.5$ K, along with an effective moment of 5.85 μ_β and a Curie–Weiss temperature of $T_{CW} = -24.48$ K, giving a frustration index of $f = |\theta_{CW}/T_N| = 3.8$. Investigation of the magnetic structure below T_N and the short-range order above T_N is ongoing.

[1] Islam, Manisha et al., Crystals 13 (2023)397
[2] Lau et al., Phys. Rev. B 80 (2009) 214414