TT 5: Correlated Electrons: Spin Systems and Itinerant Magnets – Frustrated Magnets 1 (jointly with MA)

Time: Monday 9:30–13:00 Location: H 0110

TT 5.1 Mon 9:30 H 0110

Investigation into the Magnetic Properties of Pyrochlore-type Rare-Earth Hafnates — •Jung Hwan Chun, Reinhard K. Kremer, and Chengtian Lin — MPI for Solid State Research, Stuttgart, Germany

Cubic rare-earths transition metal pyrochlores with composition $R_2TM_2O_7$ have attracted broad attention because of their unusual magnetic ground state properties related to geometrical frustration of the pyrochlores lattice. So far, the investigation focused mainly on 3*d* and 4*d* transition metal systems. The magnetic properties of rare-earths 5*d* TM pyrochlores are comparatively less well studied. Here we report on the single-crystal growth and the magnetic properties of some rare-earth hafnates (R =Nd, Gd, Dy; TM = Hf) of composition $R_2Hf_2O_7$. $Nd_2Hf_2O_7$ and $Gd_2Hf_2O_7$ crystallize with the cubic pyrochlores structure whereas diverging reports on the structure of $Dy_2Hf_2O_7$ are available in literature. Crystals of $R_2Hf_2O_7$ have been grown and their structural and magnetic properties have been investigated. Our investigations confirm $Nd_2Hf_2O_7$ and $Gd_2Hf_2O_7$ to crystallize in the cubic pyrochlores structure. Antiferromagnetic ordering below ∼0.5 K has been observed by magnetic susceptibility and heat capacity measurements for both compounds.

TT 5.2 Mon 9:45 H 0110

Finite-temperature dynamics of a highly frustrated quantum spin ladder — •Andreas Honecker[1] and Bruce Normand[2] — [1]LPTM, Université de Cergy-Pontoise, France — [2]Renmin University of China, Beijing

Highly-frustrated magnets are characterized by a (nearly) flat one-triplet excitation band at zero temperature. Little is known from theoretical studies about the temperature-dependence of this single-particle dispersion and less still concerning multi-particle dynamics at finite temperature. Experimentally, inelastic neutron scattering studies of low-dimensional frustrated systems such as $SrCu_2(BO_3)_2$ require an interpretation of the thermal evolution of scattering intensities. We investigate these issues using the example of a highly frustrated spin-1/2 ladder. We find that single- and many-particle excitations persist as sharp spectral features in the dynamic structure factor to surprisingly high and even infinite temperatures. In addition, in a relevant parameter regime low-lying excitations give rise to an anomalously rapid transfer of spectral weight out of the single-particle band to a wide range of energies.

TT 5.3 Mon 10:00 H 0110

Quantum phases of the frustrated Heisenberg model on the bilayer honeycomb lattice — •Wolfram Brenig[1], Marcelo Arlego[2], and Carlos Lamas[2] — [1]Institute for Theoretical Physics, Technical University Braunschweig, Germany — [2]IFLP - CONICET, Departamento de Física, Universidad Nacional de La Plata, Argentina

We analalyze the spin-1/2 Heisenberg antiferromagnet on the honeycomb bilayer with frustrateing next-nearest neighbor exchange. Using a combination of bond-operators, Schwinger-boson mean field theory, and dimer series expansion we evaluate and compare results for the magnetic quantum phase diagram as a function of the intra(inter) planar couplings $J_{1,2}(J_\perp)$. Evidence for both, magnetically ordered and disordered phases will be presented from results for the ground state energy, the spin gap, and real space spin-spin correlation functions. The presence of Néel, dimer, nematic, and non-collinear states will be discussed.

TT 5.4 Mon 10:15 H 0110

Spin dynamics of the bilinear-biquadratic spin-one Heisenberg model on the triangular lattice — Annika Völl and •Stefan Wessel — Institut für Theoretische Festkörperphysik, RWTH Aachen University, Germany

We study thermodynamic properties as well as the dynamical spin and quadrupolar structure factors of the O(3)-symmetric spin-1 Heisenberg model with bilinear-biquadratic exchange interactions on the triangular lattice. Based on a sign-problem-free quantum Monte Carlo approach, we access both the ferromagnetic and the ferroquadrupolar ordered, spin nematic phase as well as the SU(3)-symmetric point which separates these phases. Signatures of Goldstone soft-modes in the dynamical spin and the quadrupolar structure factors are identified, and the properties of the low-energy excitations are compared to the thermodynamic behavior observed at finite temperatures as well as to Schwinger-boson flavor-wave theory.

TT 5.5 Mon 10:30 H 0110

Quantum spin liquid in a π flux triangular lattice Hubbard model — •Stephan Rachel[1], Manuel Laubach[2], Johannes Reuther[3], and Ronny Thomale[2] — [1]Technische Universität Dresden — [2]Universität Würzburg — [3]Dahlem Center for Complex Quantum Systems and FU Berlin

We propose the π flux triangular lattice Hubbard model (π-THM) as a prototypical setup to stabilize magnetically disordered quantum states of matter in the presence of charge fluctuations. The quantum paramagnetic domain of the π-THM which we identify for intermediate Hubbard U is framed by a Dirac semi-metal for weak coupling and by 120° Néel order for strong coupling. Generalizing the Klein duality from spin Hamiltonians to tight-binding models, the π-THM maps to a Hubbard model which corresponds to the $(J_H, J_K) = (-1, 2)$ Heisenberg-Kitaev model in its strong coupling limit. The π-THM provides a promising microscopic testing ground for exotic finite-U spin liquid ground states amenable to numerical investigation.

TT 5.6 Mon 10:45 H 0110

Quantum Monte Carlo Study of Long-Range Transverse-Field Ising Models on the Triangular Lattice — •Stephan Humeniuk — Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany

Motivated by recent experiments with a Penning ion trap quantum simulator, we perform Stochastic Series Expansion quantum Monte Carlo simulations of long-range transverse-field Ising models on a triangular lattice for different decay powers α of the interactions. The phase boundary for the ferromagnet is obtained as a function of α. For antiferromagnetic interactions we find that the transverse field stabilizes a clock ordered phase with sublattice magnetization $(M, -\frac{M}{2}, -\frac{M}{2})$ with $M \approx 1$ in a process known as "order by disorder" similar to the nearest neighbour antiferromagnet on the triangular lattice. Connecting the known limiting cases of nearest neighbour and infinite-range interactions, we obtain a semi-quantitative phase diagram. Magnetization curves for the ferromagnet for experimentally relevant system sizes and with open boundary conditions are presented.

TT 5.7 Mon 11:00 H 0110

Spin liquids in kagome antiferromagnets — •Yin-Chen He, Siddhardh Morampudi, and Frank Pollmann — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187, Dresden, Germany

We propose a novel approach to describe critical spin liquids for $S = 1/2$ kagome antiferromagnets. Instead of a physical spin system, we are working on a dual model, which deals with emergent pseudo spin coupled with a compact $U(1)$ gauge field. We show that by fractionalizing the pseudo spins one can construct a class of stable deconfined critical spin liquids. This spin liquid is very different from the traditional ones, e.g., it has two different kinds of gauge field, and cannot simply be reproduced using the traditional spinon parton approach. Further, we show that a simple mean field ansatz yields an exotic critical spin liquid phase, which is described by 16 flavors of Dirac fermions coupled with one $U(1)$ and two Z_2 gauge fields. We also show such critical spin liquid can be the parent state of chiral and Z_2 spin liquids.

15 min. break.

TT 5.8 Mon 11:30 H 0110

$\mathbb{Z}_2$-vortex lattice in the ground state of Kitaev-Heisenberg models — •Maria Daghofer[1], Ioannis Rousochatzakis[2], Ulrich K Rössler[3], and Jeroen van den Brink[3] — [1]nstitut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [3]IFW Dresden, Dresden

In geometrically frustrated magnets, the strongly competing interactions between spins often suppress simple magnetic ordering patterns and clear space for new states of matter supporting rather exotic excitations, for instance, magnetic monopoles as topological excitations of spin-ice states on pyrochlore lattices. The triangular-lattice Heisenberg antiferromagnet also carries topological excitations, $\mathbb{Z}_2$ vortices, which form a $\mathbb{Z}_2$-vortex gas at finite temperatures. Here we show that spin-orbit interaction, introduced via a Kitaev term in the exchange Hamiltonian, causes the vortices to condense into a hexagonal superlattice at zero temperature. This is a new example of a nucleation transition, analogous to the Abrikosov vortex lattices in type-II superconductors, the blue phases in cholesteric liquid crystals, and the skyrmionic lattices observed in B20 chiral helimagnets. As the mechanism relies on the interplay of geometric frustration and orbital anisotropies, such vortex mesophases can materialize as a ground-state property in spin-orbit coupled correlated systems with nearly hexagonal topology, as in triangular or strongly frustrated honeycomb iridates.

TT 5.9 Mon 11:45 H 0110

Magnetic order within Kitaev–Heisenberg model — •Dorota Gotfryd[1] and Andrzej M. Oles[2,3] — [1]Institute of Theoretical Physics, Warsaw University, Pasteura 5, PL-02093 Warsaw, Poland — [2]Marian Smoluchowski Institute of Physics, Jagiellonian University, prof. S. Łojasiewicza 11, PL-30348 Kraków, Poland — [3]Max-Planck-Institut FKF, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

We present the evolution of energy spectra, spin correlation functions and order parameters for Kitaev–Heisenberg (KH) model on a single hexagon within a cluster mean-field approximation introduced in [1] in order to induce the breaking of SU(2) symmetry. The changes of these quantities are used to determine quantum phase transitions within KH model between the antiferromagnetic, stripe and Kitaev phases. In the quest of seeking physically preferred zigzag phase [2] we investigate the modifications of the phase diagram given by: (*i*) second and third neighbor Heisenberg terms, and (*ii*) anisotripic Ising-like terms added to KH Hamiltonian. We discuss the stability of this phase and possible implications for honeycomb iridates.

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[1] A. F. Albuquerque *et al.*, Phys. Rev. B **84**, 024406 (2011).
[2] J. G. Rau *et al.*, Phys. Rev. Lett. **112**, 077204 (2014).

TT 5.10 Mon 12:00 H 0110

Emergent critical phase and Z_6 order in the windmill lattice antiferromagnet — •Peter P Orth[1], Bhilahari Jeevanesan[1], Joerg Schmalian[1], Premala Chandra[2], and Piers Coleman[2] — [1]1Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08854, USA

In most systems that exhibit order at low temperatures, the order occurs in the elementary degrees of freedom such as spin or charge. Prominent examples are magnetic or superconducting states of matter. In contrast, emergent order describes the phenomenon where composite objects exhibit longer range correlations. Such emergent order has been suspected to occur in a range of correlated materials. One specific example are spin systems with competing interactions, where long-range discrete order in the relative orientation of spins may occur.

One example is the recently introduced two-dimensional antiferromagnet on the windmill lattice that shows an emergent Z_6 symmetry. The rich ground state phase diagram exhibits intricate spiral and non-coplanar phases. At finite temperature, order by disorder leads to a decoupling of an emergent collective degree of freedom given by the relative phase of spins on different sublattices. Using large scale classical parallel tempering Monte Carlo simulations, we present numerical evidence that the emergent order parameter undergoes a sequence of two Berezinskii-Kosterlitz-Thouless phase transitions that bracket a critical phase. We discuss extensions of this model and physical realizations.

TT 5.11 Mon 12:15 H 0110

The Cu^{2+} mineral szenicsite ($Cu_3(MoO_4)(OH)_4$) - a spin 1/2 J_1-J_2 chain compound with a spin gap — •Stefan Lebernegg[1], Oleg Janson[2], Alexander Tsirlin[3], and Helge Rosner[1] — [1]MPI CPfS, Dresden, Germany — [2]Institute of Solid State Physics, Vienna University of Technology, Austria — [3]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

Low-dimensional quantum magnets attracted high attention because of their exotic magnetic properties and ground states, representing an unrivaled field for challenging our understanding of collective quantum phenomena. These are governed by a complex interplay of quantum fluctuations, exchange interactions and lattice topology, which might result in magnetic frustration suppressing ordering processes. The simplest example of a frustrated system is the 1D J_1-J_2 chain with J_2 being AFM, where J_1 and J_2 are nearest- and next-nearest neighbor exchange couplings, respectively. While for an FM J_1 several materials have been discovered, for J_1 and J_2 both being AFM only very few material realizations have been found so far. In this study, we discuss the Cu^{2+}-mineral szenicsite, $Cu_3(MoO_4)(OH)_4$. A consistent microscopic magnetic model is derived from LSDA+U calculations, which can perfectly reproduce the thermodynamical data. Based on these results, an effective microscopic magnetic model is developed, demonstrating that at low temperatures szenicsite can be described in terms of an AFM J_1-J_2 chain with evidence for alternating J_2 couplings. According to the ratio $J_2/J_1 \sim 0.5$, a small spin gap should be present whose upper limit was estimated with DMRG and ED to be about 2.5 K.

TT 5.12 Mon 12:30 H 0110

The spin-1/2 Heisenberg J_1-J_2 antiferromagnet on the kagome lattice — •Yasir Iqbal[1], Didier Poilblanc[2], and Federico Becca[3] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilian's University of Würzburg, Am Hubland, D-97074, Würzburg, Germany — [2]Laboratoire de Physique Théorique UMR-5152, CNRS and Université de Toulouse, F-31062 Toulouse, France — [3]Democritos National Simulation Center, Istituto Officina dei Materiali del CNR and SISSA-International School for Advanced Studies, Via Bonomea 265, I-34136 Trieste, Italy

We report numerical calculations for the spin-1/2 Heisenberg model in presence of both nearest-neighbor J_1 and next-nearest-neighbor J_2 antiferromagnetic super-exchange couplings. Our approach is based upon Gutzwiller projected fermionic states that represents a flexible tool to describe quantum spin liquids with different properties (e.g., gapless and gapped). We show that, on finite clusters, a gapped $\mathbb{Z}_2$ spin liquid can be stabilized in presence of a finite J_2 super-exchange, with a substantial energy gain with respect to the gapless $U(1)$ Dirac spin liquid. However, this energy gain vanishes in the thermodynamic limit, implying that, at least within this approach, the $U(1)$ Dirac spin liquid remains stable in a relatively large region of the phase diagram. For $J_2/J_1 \gtrsim 0.3$, we find that a magnetically ordered state with $\mathbf{q} = \mathbf{0}$ overcomes the magnetically disordered wave functions, suggesting the end of the putative gapless spin-liquid phase.

TT 5.13 Mon 12:45 H 0110

Topological phases of interacting bosons on the kagome lattice — •Krishanu Roychowdhury[1], Subhro Bhattacharjee[2], and Frank Pollmann[3] — [1]MPIPKS, Dresden — [2]MPIPKS, Dresden — [3]MPIPKS, Dresden

We consider an extended Hubbard model of hard core bosons including nearest-neighbour hopping and long range repulsive interactions on a kagome lattice. The system is an insulator at commensurate fillings of 1/6, 1/3 and 1/2 and can be mapped to different dimer models on the triangular lattice (depending on the filling). We focus on the filling of 1/3, which transforms to a fully packed loop (FPL) model, and derive the full phase diagram in the low-energy subspace. Similar to the quantum dimer model and easy-axis kagome antiferromagnetic model studied before, we find an extended region of a gapped $\mathbb{Z}_2$ liquid with vison excitations. The gauge fluctuations, responsible for the vison modes, are dictated by the action of an *even* Ising gauge theory. In the ordered phase, where the vison gap closes, we observe a 3-fold rotationally symmetric loop ordering and present the critical theory for the amplitude fluctuations of the condensed modes. We also speculate the phase diagram for the fermionic counterpart of the model at all the above mentioned fractional fillings.