

## TT 109: Frustrated Magnets - (General) Theory

Time: Friday 9:30–12:15

Location: H 3005

TT 109.1 Fri 9:30 H 3005

**The frustrated bilayer honeycomb antiferromagnet** — ●WOLFRAM BREINIG<sup>1</sup>, MARCELO ARLEGO<sup>2</sup>, CARLOS LAMAS<sup>2</sup>, and HAO ZHANG<sup>3</sup> — <sup>1</sup>Institute for Theoretical Physics, Technical University Braunschweig, Germany — <sup>2</sup>IFLP - CONICET, Departamento de Física, Universidad Nacional de La Plata, Argentina — <sup>3</sup>National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing, China

We analyze the spin-1/2 Heisenberg antiferromagnet on the honeycomb bilayer with frustrating next-nearest neighbor exchange. Using a combination of bond-operators, Schwinger-boson mean field theory, and dimer series expansion, we show that the competition between intra- and interlayer coupling gives rise to a rich variety of semiclassical and genuinely quantum phases. Results for ground state energies, excitation gaps, and spin-spin correlation functions will be discussed. In particular we provide new evidence for the existence of a quantum disordered lattice-nematic phase within a substantial range of intermediate intralayer frustration and interlayer coupling.

TT 109.2 Fri 9:45 H 3005

**Quantum Monte Carlo Study of the Thermodynamics of the Fully Frustrated Heisenberg Bilayer** — ●STEFAN WESSEL<sup>1</sup>, JONAS STAPMANN<sup>1</sup>, ANDREAS HONECKER<sup>2</sup>, PHILIPPE CORBOZ<sup>3</sup>, BRUCE NORMAND<sup>4</sup>, and FREDERIC MILA<sup>5</sup> — <sup>1</sup>Institut für Theoretische Festkörperphysik, JARA-FIT and JARA-HPC, RWTH Aachen University, Germany — <sup>2</sup>Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, France — <sup>3</sup>Institute for Theoretical Physics and Delta Institute for Theoretical Physics, University of Amsterdam, The Netherlands — <sup>4</sup>Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Villigen, Switzerland — <sup>5</sup>Institute of Physics, Ecole Polytechnique Fédérale Lausanne (EPFL), Switzerland

We examine the thermal properties of the spin-1/2 Heisenberg model on the fully frustrated square lattice bilayer. For this purpose, we use a sign problem-free quantum Monte Carlo approach that is based on a decoupling of the Hamiltonian in an inter-layer spin dimer basis. At zero temperature, a discontinuous quantum phase transition separates a inter-layer singlet phase from an antiferromagnetic ground state forming from inter-layer triplet states. We show that this discontinuous transition extends towards finite temperatures, i.e., in the absence of long-range order. The thermodynamic behavior of this system furthermore exhibits similarities to the liquid-gas transition.

TT 109.3 Fri 10:00 H 3005

**Cluster-glass phase in pyrochlore XY antiferromagnets with quenched disorder** — ●MATTHIAS VOJTA<sup>1</sup>, JOSE A. HOYOS<sup>2</sup>, ERIC C. ANDRADE<sup>2</sup>, and STEPHAN RACHEL<sup>1,3</sup> — <sup>1</sup>Technische Universität Dresden, Germany — <sup>2</sup>Universidade de Sao Paulo, Brasil — <sup>3</sup>University of Melbourne, Australia

We study the impact of quenched disorder (random exchange couplings or site dilution) on easy-plane pyrochlore antiferromagnets. In the clean system a magnetically ordered state is selected from a classically degenerate manifold via an order-by-disorder mechanism. In the presence of randomness, however, different states can be locally selected depending on details of the disorder configuration. Using a combination of analytical considerations and classical Monte-Carlo simulations, we argue that any long-range-ordered magnetic state is destroyed beyond a critical level of randomness where the system breaks into magnetic domains due to random exchange anisotropies, becoming therefore a glass of spin clusters, in accordance with the available experimental data.

TT 109.4 Fri 10:15 H 3005

**Quenched bond disorder in a non-collinear antiferromagnet** — ●SANTANU DEY and MATTHIAS VOJTA — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

In antiferromagnets, the presence of geometric frustration often leads to classical ground states with non-collinear spin ordering. Quenched disorder is an interesting ingredient which tends to counteract spontaneous symmetry breaking in low dimensional systems. Consequently, the study of the interplay between disorder and frustration has garnered some serious attention recently [1,2]. To understand the resulting

phenomena, we undertake a generic point of view and also focus on a prototypical example, the disordered triangular lattice antiferromagnet (TLAF) with next and next to nearest neighbor Heisenberg interaction. The homogeneous limit of this model hosts a phase transition between non-collinear antiferromagnetic LRO and what is believed to be a  $\mathbb{Z}_2$  spin liquid [3]. Combining analytical arguments and finite-system numerical simulations, we study the destruction of the LRO by bond disorder and discuss physical properties of the emergent state at low temperatures. We also connect our findings to recent experimental observations on related compounds, YbZnGaO<sub>4</sub> and YbMgGaO<sub>4</sub> [1]. [1] Z. Ma et. al, arXiv:1709.00256 (2017) [2] H. Kawamura, K. Watanabe, T. Shimokawa, J. Phys. Soc. Jpn. 83, 103704 (2014) [3] K. Slagle and C. Xu, Phys. Rev. B. 89, 104418 (2014)

TT 109.5 Fri 10:30 H 3005

**Frustrated quantum magnetism in the Kondo-lattice on the zig-zag ladder** — ●MATTHIAS PESCHKE, ROMAN RAUSCH, and MICHAEL POTTHOFF — I. Institut für Theoretische Physik, Universität Hamburg

The interplay between Kondo effect, indirect magnetic interaction and geometrical frustration is studied in the Kondo lattice on the one-dimensional zig-zag ladder. Using the density-matrix renormalization group (DMRG), the ground state and various short- and long-range spin- and density-correlation functions are calculated for the model at half-filling as a function of the antiferromagnetic Kondo interaction down to  $J = 0.3t$  where  $t$  is the nearest-neighbor hopping.

Geometrical frustration is shown to lead to at least two critical points: Starting from the strong- $J$  limit, where almost local Kondo screening dominates, antiferromagnetic correlations between nearest-neighbor and next-nearest-neighbor local spins become stronger and stronger, until at  $J_c^{\text{dim}} \approx 0.895$  frustration is alleviated by a spontaneous breaking of translational symmetry and a corresponding transition to a dimerized state. Furthermore, within the symmetry-broken dimerized state, our data suggest a magnetic transition to a  $90^\circ$  quantum spin spiral with quasi-long-range order at  $J_c^{\text{mag}} \approx 0.84$ . The quantum-critical point is characterized by a diverging spin-structure factor  $S(q)$  at wave vector  $q = \pi/2$  and the closure of the spin gap (based on system sizes up to  $L = 40$ ). This is opposed to the model on the one-dimensional bipartite chain, which is known to have a finite spin gap for all  $J > 0$  at half-filling.

TT 109.6 Fri 10:45 H 3005

**Quantum criticality of 2d transverse-field Ising models with long-range interactions** — SEBASTIAN FEY and ●KAI P. SCHMIDT — Lehrstuhl für Theoretische Physik I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Most investigations on strongly correlated quantum many-body systems tackle short-range interactions. Very little is known so far on quantum criticality in the presence of long-range interactions, since such models are very hard to treat microscopically. Nevertheless, important examples of long-range interactions exist in nature, e.g. dipolar interactions in spin ice or long-range forces between cold atoms in optical lattices. Here we develop linked-cluster expansions with the help of classical Monte Carlo simulations to investigate the quantum-critical properties of the transverse-field Ising model with long-range interactions on two-dimensional lattices. In the unfrustrated cases we find different kinds of universality classes corresponding to the nearest-neighbor model, mean-field theory, as well as continuously varying critical exponents. In the frustrated cases our results agree with the scenario that the quantum-critical properties are always given by the model with nearest-neighbor interactions.

TT 109.7 Fri 11:00 H 3005

**$\mathbb{Z}_2$  Topological quantum paramagnet on a honeycomb bilayer** — ●DARSHAN G. JOSHI and ANDREAS P. SCHNYDER — Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Topological quantum paramagnets are exotic states of matter with trivial paramagnetic ground states hosting topological excitations. Here we show that a simple model of quantum spins on a honeycomb bilayer hosts a  $\mathbb{Z}_2$  topological quantum paramagnet in the presence of spin-orbit coupling. The  $\mathbb{Z}_2$  invariant is the same as that in the case

of the fermionic quantum spin Hall state. We further show that upon making one of the Heisenberg couplings stronger the system undergoes a topological quantum phase transition, where the  $\mathbb{Z}_2$  invariant vanishes, to a different topological quantum paramagnet. In this case the edge states are disconnected from the bulk excitations and the phase is characterized by a different topological invariant. This physics is amenable to experiments, where an anisotropic coupling can be induced under pressure.

15 min. break.

TT 109.8 Fri 11:30 H 3005

**Thermodynamics of the Two-Dimensional Shastry-Sutherland Model for  $\text{SrCu}_2(\text{BO}_3)_2$**  — ●ANDREAS HONECKER<sup>1</sup>, JONAS STAPMANN<sup>2</sup>, IDO NIESEN<sup>3</sup>, PHILIPPE CORBOZ<sup>3</sup>, BRUCE NORMAND<sup>4</sup>, FRÉDÉRIC MILA<sup>5</sup>, and STEFAN WESSEL<sup>2</sup> — <sup>1</sup>Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, France — <sup>2</sup>Institut für Theoretische Festkörperphysik, JARA-FIT and JARA-HPC, RWTH Aachen University, Germany — <sup>3</sup>Institute for Theoretical Physics and Delta Institute for Theoretical Physics, University of Amsterdam, The Netherlands — <sup>4</sup>Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Villigen, Switzerland — <sup>5</sup>Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

$\text{SrCu}_2(\text{BO}_3)_2$  is famous for its rich physical properties and as a realization of the two-dimensional spin-1/2 Shastry-Sutherland model. In the latter model, an orthogonal arrangement of dimers gives rise both to an exact dimer ground state and geometric frustration that renders quantitatively reliable results for the low-temperature thermodynamic properties a challenge since, e.g., conventional Quantum-Monte-Carlo (QMC) simulations suffer from a severe sign problem. A recently developed QMC method in the dimer basis alleviates the sign problem. We assess the range of applicability of this method to the two-dimensional spin-1/2 Shastry-Sutherland model by comparing it to complementary exact diagonalization and high-temperature series. Specifically, we compute the specific heat  $C$  and the magnetic susceptibility  $\chi$  in the parameter regime relevant to  $\text{SrCu}_2(\text{BO}_3)_2$ .

TT 109.9 Fri 11:45 H 3005

**Plaquette phases in an extended Shastry-Sutherland model** —

●CAROLIN BOOS<sup>1</sup>, PHILIPPE CORBOZ<sup>2</sup>, SCHELTO CRONE<sup>2</sup>, FRÉDÉRIC MILA<sup>3</sup>, IDO NIESEN<sup>2</sup>, and KAI PHILLIP SCHMIDT<sup>1</sup> — <sup>1</sup>FAU Erlangen-Nürnberg, Germany — <sup>2</sup>University of Amsterdam, Netherlands — <sup>3</sup>EPF Lausanne, Switzerland

The frustrated magnet  $\text{SrCu}_2(\text{BO}_3)_2$  exhibits a quantum phase transition under high pressure. Without pressure this material is well described by the two-dimensional Shastry-Sutherland model with parameters close to a phase transition towards a ground state of singlets on empty plaquettes. This state is therefore the natural candidate for the high-pressure phase. However, it has also been suggested [1] that a different plaquette phase, where singlets reside on the full plaquettes containing a diagonal bond, is realized in  $\text{SrCu}_2(\text{BO}_3)_2$ . In this work we use high-order series expansions and infinite projected entangled pair states (iPEPS) to investigate the interplay between empty and full plaquette phases in an extended Shastry-Sutherland model.

[1] M. E. Zayed *et al.*, Nat. Phys. **13** (2017) 962

TT 109.10 Fri 12:00 H 3005

**Spin model of the Heisenberg antiferromagnet  $\text{Li}_3\text{Ni}_2\text{SbO}_6$ : the relevance of third-neighbor exchanges** — ●OLEG JANSON — Institut für Festkörperphysik, TU Wien, Österreich

The quasi-2D  $S=1$  Heisenberg antiferromagnet  $\text{Li}_3\text{Ni}_2\text{SbO}_6$  exhibits a small Weiss temperature of 8 K and a zigzag magnetic ground state below  $T_N=15$  K [1,2]. At the same time, the experiments indicate the presence of a short-range magnetic order up to 80 K [2]. The experimental behavior was rationalized in terms of a honeycomb lattice model with inequivalent nearest-neighbor (NN) exchanges [1]: antiferromagnetic  $J_1$  forming dimers and ferromagnetic  $J'_1$  ( $J_2$  in the notation of [1]) forming chains. Puzzled by the drastic dissimilarity of  $J_1$  and  $J'_1$ , we performed microscopic magnetic modeling and found that both NN exchanges are ferromagnetic. The antiferromagnetism and magnetic frustration are induced by two sizable third-neighbor exchanges,  $J_3$  and  $J'_3$ , that are mediated by the nonmagnetic  $\text{SbO}_6$  octahedra in the voids of the honeycomb lattice. The resulting  $J_1$ - $J'_1$ - $J_3$ - $J'_3$  model provides a simple and natural explanation for the observed zigzag state. This work has been supported by the Austrian Science Fund (FWF) through the Lise Meitner programme, project no. M2050.

[1] E. A. Zvereva *et al.*, Phys. Rev. B **92**, 144401 (2015).

[2] A. I. Kurbakov *et al.*, Phys. Rev. B **96**, 024417 (2017).