TT 23: Frustrated Magnets - General 1 (joint session TT/MA)

Time: Tuesday 9:30–13:00 Location: Theater

TT 23.1 Tue 9:30 Theater

Ground state properties of the sawtooth chain — •Alexandros Metavitsiadis and Wolfram Brenig — Institute for Theoretical Physics, TU Braunschweig, 38106 Braunschweig, Germany

Recent experimental and theoretical studies on the natural mineral Atacamite [$Cu_2Cl(OH)_3$] have revealed that it might be one of the few true cases where a sawtooth chain, a minimal one-dimensional frustrated system, is materialized. Prompted by these recent results, we revisit the low energy properties of the sawtooth chain presenting a comprehensive theoretical study of its ground state properties using numerical techniques (full diagonalization, Lanczos, and matrix product states), as well as analytical field theory calculations.

TT 23.2 Tue 9:45 Theater

Magnetization plateau in the frustrated quantum sawtooth chain atacamite, $Cu_2Cl(OH)_3$ — •Leonie Heinze[1], Xiaxin Ding[2], Vivien Zapf[2], Franziska Weickert[2], Marcelo Jaime[2], Gaël Bastien[3], Anja U.B. Wolter[3], Manfred Reehuis[4], Jens-Uwe Hoffmann[4], Ralf Feyerherm[4], Dirk Menzel[1], Kirrily C. Rule[5], and Stefan Süllow[1] — [1]IPKM, TU Braunschweig, Braunschweig, Germany — [2]NHMFL, Los Alamos, USA — [3]IFW Dresden, Dresden, Germany — [4]HZB, Berlin, Germany — [5]ANSTO, Kirrawee, Australia

The frustrated nature of the quantum magnet atacamite, $Cu_2Cl(OH)_3$, is displayed by its magnetic properties [1]. Band structure calculations [2] suggest that the magnetic coupling scheme can essentially be understood in terms of a quantum sawtooth chain with a dominant coupling along the chain of about $J_1 \sim 100\,\mathrm{K}$, and a secondary coupling about $J_2 \sim 30\,\mathrm{K}$.

Here, we present new insights into the magnetic phase diagram of atacamite. We discuss the long-range ordered magnetic ground state below $T_\mathrm{N} = 8.6\,\mathrm{K}$ and present high field magnetization data revealing a 1/2-magnetization plateau. Magnetic saturation is estimated to be attained in fields between 75 to 80 T.

[1] L. Heinze, *et al.*, Physica B **536**, 377 (2018)
[2] H. O. Jeschke and R. Valentí, private communication.

TT 23.3 Tue 10:00 Theater

Phase diagram of the pseudo-Kagome francisite $Cu_3Bi(SeO_3)_2O_2Cl$ studied by high-resolution dilatometry — •Sven Spachmann[1], Liran Wang[1], Alexander Vasiliev[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Lomonosov Moscow State University, Moscow, Russia

Single crystals of the layered Kagome-like francisite $Cu_3Bi(SeO_3)_2O_2Cl$ have been studied by high-resolution thermal expansion and magnetostriction as well as by bulk magnetization measurements. At $B = 0$ T, in addition to a well-known structural phase transition at $T_\mathrm{s} = 120$ K, long range antiferromagnetic order of the ferromagnetically coupled layers develops around $T_\mathrm{N} = 26.4$ K. The ordering is associated with pronounced anomalies in the uniaxial thermal expansion coefficients. Magnetic fields yield a suppression of T_N. In plane, a sign change of the uniaxial pressure dependencies (at $B > 2$ T for $B \| a$) signals a change in the nature of the phase transition. At $T = 2$ K, metamagnetic transitions are observed for B parallel to the (in-plane) a-, b-, and (out-of-plane) c-axes at $B_\mathrm{C} = 5.4$ T, 1.6 T, and 0.9 T, respectively. The transitions are associated with sharp magnetization jumps. The magnetic phase diagram for all three crystal axes is constructed and discussed.

TT 23.4 Tue 10:15 Theater

Magnetic excitations in the correlated paramagnetic state of the frustrated quantum antiferromagnet Cs_2CuCl_4 — •Bernd Wolf, Paul Eibisch, Lars Postulka, Franz Ritter, Cornelius Krellner, and Michael Lang — Physikalisches Institut, Goethe Universität, SFB/TR49, D-60438 Frankfurt (M)

We present a magnetoelastic investigation of the frustrated triangular-lattice S = 1/2 antiferromagnet Cs_2CuCl_4 by studying the longitudinal modes c_{11}, c_{22} and c_{33}. The measurements were performed in magnetic fields up to 10 T and down to 0.032 K to cover the the long range order and the spin-liquid regime. At the lowest temperatures of our experiment the field dependence of the c_{33} mode can be well described using a Landau free energy model which combines the elastic constant with the magnetic susceptibility data, measured independently. From fits to the experimental c_{33} data we obtain a very small magnetoelastic coupling constant $G/k_B = 2.8\,\mathrm{K}$ for Cs_2CuCl_4 consistent with the results of susceptibility measurements under hydrostatic pressure. Remarkably, we find that the classical approach provides an excellent description of the data at lowest temperatures, i.e., close to the putative quantum critical point at B = 8.5 T of this material. However, at somewhat higher temperatures, there are deviations between the experimental data and the theoretical curves. At these temperatures we also observe anomalies in the ultrasonic attenuation α and χ'', the imaginary part of the magnetic susceptibility. We discuss these losses with respect to the peculiarities of the magnetic excitation spectrum for this low dimensional spin system.

TT 23.5 Tue 10:30 Theater

Thermodynamics of the 2D $S = 1/2$ Shastry-Sutherland Model and $SrCu_2(BO_3)_2$ — Alexander Wietek[1], Philippe Corboz[2], Frédéric Mila[3], Bruce Normand[4], Stefan Wessel[5], and •Andreas Honecker[6] — [1]Center for Computational Quantum Physics, Flatiron Institute, New York, USA — [2]Institute for Theoretical Physics and Delta Institute for Theoretical Physics, University of Amsterdam, The Netherlands — [3]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland — [4]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Switzerland — [5]Institut für Theoretische Festkörperphysik, RWTH Aachen University, Germany — [6]Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, France

Reliable computation of the low-temperature thermodynamic properties of highly frustrated quantum magnets such as the 2D $S = 1/2$ Shastry-Sutherland model is a considerable challenge. Notwithstanding recent progress with QMC simulations in the dimer basis, the parameter regime relevant to $SrCu_2(BO_3)_2$ has remained inaccessible [1]. Here we present accurate results obtained from two other methods, namely Thermal Pure Quantum (TPQ) states and infinite Projected Entangled Pair States (iPEPS). We observe the emergence of a low-temperature peak in the specific heat C and relate it to the large number of bound states that emerge close to the first-order transition from the dimer to the plaquette phase.

[1] S. Wessel, I. Niesen, J. Stapmanns, B. Normand, F. Mila, P. Corboz, A. Honecker, Phys. Rev. B **98**, 174432 (2018)

TT 23.6 Tue 10:45 Theater

Theory of the intermediate phase of $SrCu_2(BO_3)_2$ under pressure — •Carolin Boos[1,2], Schelto Crone[3], Ido Niesen[3], Philippe Corboz[3], Frédéric Mila[2], and Kai Phillip Schmidt[1] — [1]FAU Erlangen-Nürnberg, Germany — [2]EPF Lausanne, Switzerland — [3]University of Amsterdam, Netherlands

Building on the NMR evidence that two different Cu sites are present in the intermediate phase of $SrCu_2(BO_3)_2$ under pressure, we investigate the nature of the intermediate phase in an orthorhombically distorted Shastry-Sutherland model. We show that a few percent difference between nearest-neighbor couplings is sufficient to destabilize the plaquette phase in favor of a one-dimensional phase in which bonds around half the full plaquettes become stronger. This phase is adiabatically connected to the Haldane phase that is stabilized when next-nearest neighbor couplings take different values, and the excitations in this one-dimensional phase are shown to agree qualitatively with neutron scattering results.

TT 23.7 Tue 11:00 Theater

Electron spin resonance studies on the frustrated tripod-Kagome compound $Mg_2Gd_3Sb_3O_{14}$ — •Christoph Wellm[1,2], Julian Zeisner[1,2], Mihai Sturza[1], Gaël Bastien[1,2], Sebastian Gass[1], Anja U.B. Wolter[1], Bernd Büchner[1,2], and Vladislav Kataev[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 — [2]Institut für Festkörper-und Materialphysik, TU Dresden, D-01062

As an example of a class of geometrically frustrated magnetic systems, the so-called tripod Kagome materials have been suggested as an interesting target of experimental investigation due to the frustrated nature and the question of dimensionality of the magnetic interactions. In our work we performed high-field electron spin resonance measurements on

a powder sample of $Mg_2Gd_3Sb_3O_{14}$, a representative of a quasiclassical Heisenberg magnet, where the effect of spin-orbit coupling of Gd^{3+} ions vanishes to first order. Measurements were conducted over a frequency range of 70-420 GHz and temperatures ranging from 3-50 K. The Gaussian lineshape is consistent with a model of dominant dipolar spin-spin interactions, while the growing asymmetry of the lineshape upon decrease of temperature signifies an increase of an effective internal field, an indication of increasing short-range spin-spin-correlations. Such a behavior is typical for frustrated systems, making our studies one of the first to reveal such significant features in this family of materials. Furthermore, temperature dependent critical broadening of the linewidth and increase of the internal field strength provide insights into the dimensionality of the spin-spin correlations.

15 min. break.

TT 23.8 Tue 11:30 Theater

Frustrated magnetism of S=5/2 moments on a coupled triangular lattice in $Cs_3Fe_2Br_9$ — •Daniel Brüning[1], Tobias Fröhlich[1], Markus Braden[1], Ladislav Bohatý[2], Petra Becker[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Deutschland — [2]Abteilung Kristallographie, Institut für Geologie und Mineralogie, Universität zu Köln, Deutschland

$Cs_3Fe_2Br_9$ is a hexagonal material consisting of Fe^{3+} ions with S=5/2 in face-sharing Fe_2Br_9 bi-octahedra, which form hexagonal double layers of the Fe ions. The triangular arrangement of the magnetic ions in the individual layers causes magnetic frustration. The type of magnetic ground state depends on the ratio between the magnetic exchange couplings: the intradimer coupling J, the intralayer (or in-plane) coupling J_p, and the interlayer coupling J_c. The magnetic ground state of $Cs_3Fe_2Br_9$ is not a singlet-dimer state as in isostructural $Cs_3Cr_2Br_9$ and $Cs_3Cr_2Cl_9$, but there is evidence for antiferromagnetic order with $T_N = 13.5$ K. However, our measurements up to 17 T on large single crystals reveal a very unusual magnetic field vs. temperature phase diagram. For an in-plane field, we find linear M(H) curves, whereas a field H‖c causes multiple phase transitions including a magnetization plateau of 1/3 $M_{sat} = 10\mu_B$. Neutron diffraction resolved the magnetic structure of two phases which indicate an increasing intralayer coupling. Additionally, we present pulsed-field magnetization measurements revealing further transitions, before reaching saturation around 40 T for H‖c.

This work was supported by the DFG through CRC 1238.

TT 23.9 Tue 11:45 Theater

Importance of biquadratic exchange for a new Ni-based quantum magnet of frustrated $S = 1$ isolated spin-triangles — •B Lenz[1], S Chattopadhyay[2], S Kanungo[3], NA Sushila[4], S K Panda[1], S Biermann[1,5], W Schnelle[6], K Manna[2], R Kataria[4], M Uhlarz[2], Y Skourski[2], S A Zvyagin[2], A Ponomaryov[2], T Herrmannsdörfer[2], R Patra[4], and J Wosnitza[2,7] — [1]CPHT, Ecole Polytechnique, Palaiseau, France — [2]Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, Germany — [3]School of Physical Sciences, IIT Goa, India — [4]Department of Chemistry and Centre for Advanced Studies in Chemistry, Panjab University, India — [5]Collège de France, Paris, France — [6]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [7]Institut für Festkörper- und Materialphysik, TU Dresden, Germany

The new metal-organic framework BHAP-Ni_3 is comprised of essentially isolated spin-1 triangle centers, which renders this quantum magnet an ideal system to study the magnetism of a frustrated spin-triangle unit. Pulsed-field magnetometry and AC-susceptibility measurements of single-crystalline samples allow to identify a disordered magnetic ground state and a peculiar pronounced 2/3 magnetization plateau between 7T and 20T. Here, we show how theoretical modeling guided by ab initio calculations identifies the interplay of Heisenberg and biquadratic spin-spin interactions to be responsible for the stabilization of an exotic state that manifests itself in form of the 2/3 magnetization plateau.

TT 23.10 Tue 12:00 Theater

Estimating the density of states of frustrated spin systems — •Martin Weigel[1], Lev Barash[2], Jeffrey Marshall[3], and Itay Hen[3] — [1]Applied Mathematics Research Centre, Coventry University, Priory Street, Coventry, CV1 5FB, UK — [2]Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia — [3]Department of Physics and Astronomy, and Center for Quantum Information Science & Technology, University of Southern California, Los Angeles, California 90089, USA

Estimating the density of states of systems with rugged free energy landscapes is a notoriously difficult task of the utmost importance in many areas of physics ranging from spin glasses to biopolymers. Density of states estimation has also recently become an indispensable tool for the benchmarking of quantum annealers when these function as samplers. Some of the standard approaches suffer from a spurious convergence of the estimates to metastable minima, and these cases are particularly hard to detect. Here, we introduce a sampling technique based on population annealing enhanced with a multi-histogram analysis and report on its performance for spin glasses. We demonstrate its ability to overcome the pitfalls of other entropic samplers, resulting in some cases in orders of magnitude scaling advantages that can result in the uncovering of new physics. To do that we devise several schemes that allow us to achieve exact counts of the degeneracies of the tested instances.

TT 23.11 Tue 12:15 Theater

Ground states of the transverse-field long-range Ising model on infinite-cylinder triangular lattices — •Jan Koziol, Sebastian Fey, and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, Staudtstraße 7, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

To gain a better understanding of the interplay between frustrated long-range interactions and zero-temperature quantum fluctuations, we investigate the ground-state phase diagram of the transverse-field Ising model with algebraically-decaying long-range Ising interactions on quasi one-dimensional infinite-cylinder triangular lattices. Technically, we apply various approaches including low-field and high-field series expansions. For the classical long-range Ising model, we investigate cylindric triangular lattice configurations, i.e. a triangular lattice with an even finite length periodic boundary condition ($4 - 40$ lattice sites) in one direction and infinite extension in the other direction. We show the occurrence of new columnar-ordered phases differing from the infinitely degenerate nearest-neighbour Ising ground-state manifold on the two-dimensional triangular lattice. The existence of these columnar phases is connected to the long-range nature of the Ising interaction. For the full quantum model, we concentrate on cylinders with extensions four and six. The ground-state phase diagram consists of several quantum phases in both cases including a polarised phase, columnar-ordered phases, and ordered phases which emerge from an order by disorder scenario already present in the nearest-neighbour model.

TT 23.12 Tue 12:30 Theater

Quantum-criticality in two-dimensional transverse-field Ising models with frustrated long-range interactions — •Sebastian Fey, Sebastian C. Kapfer, and Kai P. Schmidt — FAU Erlangen-Nürnberg, Germany

Quantum-critical behavior is found in many quantum systems displaying universal properties such as critical exponents. In the past, most investigations of strongly correlated quantum many-body systems have tackled short-range interactions because long-range interacting systems are notoriously difficult to treat. 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 present results for the frustrated long-range transverse-field Ising model (lrTFIM) with antiferromagnetic interactions on two-dimensional lattices obtained via linked-cluster expansions extended by classical Monte-Carlo integrations. It is found that the nature of the phase transition crucially depends on the lattice geometry: On the square lattice, the lrTFIM remains in the nearest-neighbor universality class for all algebraically-decaying interactions studied. In contrast, on the triangular lattice, the nature of the quantum phase transition changes from 3D XY universality to a first-order transition due to the presence of a stripe-ordered phase for very slowly-decaying Ising interactions.

TT 23.13 Tue 12:45 Theater

Magnetism of the N = 42 kagome lattice antiferromagnet — •Jürgen Schnack[1], Jörg Schulenburg[2], and Johannes Richter[3] — [1]Fakultät für Physik, Universität Bielefeld, Postfach 100131, D-33501 Bielefeld, Germany — [2]Universitätsrechenzentrum, Universität Magdeburg, D-39016 Magdeburg, Germany — [3]Institut für Physik, Universität Magdeburg, P.O. Box 4120, D-39016 Magdeburg, Germany and Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

For the paradigmatic frustrated spin-half Heisenberg antiferromagnet on the kagome lattice we performed large-scale numerical investigations of thermodynamic functions by means of the finite-temperature Lanczos method for system sizes of up to N = 42 [1]. We present the dependence of magnetization as well as specific heat on temperature and external field and show in particular that a finite-size scaling of specific heat supports the appearance of a low-temperature shoulder below the major maximum. This seems to be the result of a counterintuitive motion of the density of singlet states towards higher energies. Other interesting features that we discuss are the asymmetric melting of the 1/3 magnetization plateau as well the field dependence of the specific heat that exhibits characteristic features caused by the existence of a flat one-magnon band. By comparison with the unfrustrated square-lattice antiferromagnet the tremendous role of frustration in a wide temperature range is illustrated.

[1] Phys. Rev. B 98, 094423 (2018)