

AGJDPG 1: PhD Symposium: Quantum Magnets: Frustration and Topology in Experiment and Theory (jointly with MA)

Organizers: Boris Celan, Leonie Heinze, Niklas Casper, Jonas Richter, Benjamin Köhler (TU Braunschweig)

Quantum magnetism is a very active area of condensed matter physics. In the last decades, this fascinating field has highly profited from the fruitful interplay of experiment and theory. It is a genuinely interdisciplinary area of research, linking across many different subfield boundaries, ranging from condensed matter and statistical physics, via ultra cold atomic gases, spin- and heat caloritronics, classical and quantum information theory, to questions in material design and device technology. Frustrated quantum magnets can be realized in spin systems in which localized magnetic moments interact through competing exchange interactions that cannot be simultaneously satisfied. Such spin systems may be frustrated due to a multitude of reasons, e. g., quantum chemistry can lead to competing exchange paths or lattice geometry can induce frustration. Furthermore, spin-orbit interactions may lead to pseudo-spins with frustrating compass interactions and higher-order exchange can generate frustration through ring exchange. On the classical level frustration gives rise to a large degeneracy of the system ground state. Frustration occurs due to geometrical reasons or higher order exchange processes. On the quantum level this might lead to the emergence of unconventional solid and liquid phases with exotic excitations. In this context, the possibility of spin liquids is quite interesting from a theoretical as well as from an experimental point of view. While in early days spin liquids have merely been considered to be magnets which lack any type of long range order down to $T=0$, it has only been realized very recently that such liquids are a novel form of correlated matter which shows topological order and intimately linked to that, fractionalized excitations. In theory, the formation of such matter defies a description in terms of standard Ginzburg-Landau theory and it seems fair to say, that its physics is far from being understood. In experiment, first potentially promising candidates may have been synthesized, such as e. g. triangular magnets in organics, quantum spin ice on pyrochlores, and Kitaev model variants in iridates. Yet, the search for definite materials is still ongoing. All in all, the study of frustrated quantum magnets reveals new physics and generates contributions to the development of novel materials. The investigation of quantum magnets is however a challenging problem. On the theoretical side numerous sophisticated methods have been developed and applied to gain insight into the properties of spin models, e. g. emergent gauge, and topological field theories, DMRG methods, tensor networks, variational Monte-Carlo and others. On the experimental side extensive material design has to be combined with a multitude of state-of-art probes, like nuclear magnetic resonance (NMR) and muon spin resonance (μ -SR), RIXS, INS, Raman, electron and tunneling spectroscopies as well as transport, high magnetic field, and thermodynamic measurements in order to identify potentially interesting compounds.

Time: Tuesday 9:30–15:00

Location: HSZ 04

Welcome and Introduction

Invited Talk AGJDPG 1.1 Tue 9:45 HSZ 04
Frustrated Quantum Magnets: Theory — ●MATTHIAS VOJTA —
 Technische Universität Dresden, Germany

This tutorial will cover theoretical concepts of frustrated magnetism. It will start from the classical degeneracies induced by strong geometric frustration, discuss order-by-disorder phenomena, and lay out ideas for quantum spin liquids. The emergence of fractionalized excitations and artificial gauge fields will be discussed using explicit microscopic models. Physical signatures of these emergent phenomena will be highlighted. Further topics will include frustration in metallic systems, quantum phase transitions in the presence of frustration, and the role of quenched disorder. Throughout the talk, links to concrete materials will be pointed out.

Invited Talk AGJDPG 1.2 Tue 10:30 HSZ 04
Ground State Selection in Quantum Pyrochlore Magnets
 — ●BRUCE D. GAULIN — McMaster University, Hamilton, Ontario,
 Canada

Rare-earth (RE) based cubic pyrochlore magnets, with composition $\text{RE}_2\text{B}_2\text{O}_7$, are characterized by having RE^{3+} ions decorate a network of corner-sharing tetrahedra, one of the canonical architectures supporting geometric frustration in three dimensions. For a given $\text{RE}_2\text{B}_2\text{O}_7$ series, such as with the non-magnetic $\text{B}=\text{Ti}^{4+}$, crystalline electric field effects give different anisotropies for the magnetic RE ion, while varying crystal chemistry results in different magnetic interactions. The combination of these two produces a remarkable diversity of exotic magnetic ground states across a series such as $\text{RE}_2\text{Ti}_2\text{O}_7$. I will describe this series of materials, and point out how local XY

anisotropy gives rise to $S_{\text{effective}}=1/2$ quantum spins for $\text{Yb}_2\text{Ti}_2\text{O}_7$ and $\text{Er}_2\text{Ti}_2\text{O}_7$. These two quantum pyrochlore magnets display very different ground states, a highly disordered, candidate quantum spin ice state in $\text{Yb}_2\text{Ti}_2\text{O}_7$, and a non-linear Neel state selected by the "order-by-disorder" mechanism for $\text{Er}_2\text{Ti}_2\text{O}_7$, due to their net ferromagnetic and antiferromagnetic interactions, respectively. I will focus mainly on experimental techniques, principally neutron scattering and heat capacity measurements, that can provide microscopic information on both the ground state and the excitations within the exotic ground states which these materials display.

15 min. break

Invited Talk AGJDPG 1.3 Tue 11:30 HSZ 04
Effects of anisotropic exchange in strong spin-orbit coupled magnets — ●NATALIA PERKINS — University of Minnesota, Minneapolis, USA

Recently, the Jackeli-Khaliullin Kitaev (JKK) materials on various two- and three-dimensional tri-coordinated lattices, which are believed to be proximate to the Kitaev Quantum spin liquid, have attracted a lot of attention. In all these materials, the geometry of the lattices with edge-sharing octahedra of ligand ions is such that it gives rise to the dominant Kitaev interactions between effective $j=1/2$ magnetic moments of the transition metal ions. Nevertheless, the experimental studies of the JKK materials have shown that at sufficiently low temperatures and ambient pressure all of them order magnetically. These findings suggest that experimentally relevant super-exchange models must contain other subdominant interactions between magnetic moments in addition to the Kitaev coupling. In my talk I will discuss the effects of these anisotropies. I will show that the Kitaev spin liquid is

very fragile with respect to the both second neighbor Kitaev interaction and the off-diagonal symmetric exchange anisotropy. I will also show that the off-diagonal exchange anisotropy drives the model to a classical spin liquid phase, characterized by an extensive number of ground states and ultra-short, highly anisotropic spin-spin correlations.

Invited Talk AGjDPG 1.4 Tue 12:00 HSZ 04
Numerical Approaches to Frustrated Quantum Magnets —
 ●STEPHAN RACHEL — Institute for Theoretical Physics, TU Dresden, Germany

Frustrated magnetism is one of the most vibrant and exciting fields of modern condensed matter physics. In particular, frustrated magnets are the hiding places of quantum spin liquids, a state of matter which does not exhibit magnetic long-range order but which possesses fractionalized elementary excitations. In this talk, I will give an overview of the numerical methods available for the investigation of frustrated magnets and discuss advantages and limitations. In particular, I will focus on recent developments for the investigation of three-dimensional quantum magnets and the search of spin liquid states.

AGjDPG 1.5 Tue 12:30 HSZ 04
Thermal and spin transport properties of frustrated spin-1/2 chains in high magnetic fields — ●JAN STOLPP¹, CHRISTOPH KARRASCH², SHANG-SHUN ZHANG³, CRISTIAN BATISTA³, and FABIAN HEIDRICH-MEISNER¹ — ¹Arnold Sommerfeld Center for Theoretical Physics - Ludwig-Maximilians-Universität München — ²Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin — ³Department of Physics, University of Tennessee, Knoxville, and Oak Ridge National Laboratory

We perform a full diagonalization study of frustrated spin-1/2 chains (i.e. spin-1/2 chains with nearest and next nearest neighbor interaction) in the presence of an external magnetic field. The thermal and spin conductivity are computed from Kubo formulae as a function of frustration and field strength. We are especially interested in the transport properties in the vector chiral phase that appears in the phase diagram at strong frustration and in a high field. We observe an enhanced low-frequency response in the high-field vector chiral phase which we trace back to a renormalization and enhancement of the characteristic velocity.

Lunch break

Invited Talk AGjDPG 1.6 Tue 13:45 HSZ 04
Nuclear Probes on Frustrated Magnets — ●PHILIPPE MENDELS — Lab. Physique des Solides, Univ. Paris-Sud, Orsay, France

NMR and μ SR are two local powerful probes which often complement thermodynamic and neutron studies. I will first briefly introduce these two techniques and the parameter ranges (pressure, temperature, field) in which they can operate. I will then show how they give access to im-

portant information in the case of frustrated magnets: magnetic ordering, phase diagrams and magnetic fluctuations, spin liquid phases, field induced spin textures, opening of spin gaps. This will cover various up to date cases, triangular magnets, quantum spin ice, spin liquids... In the last part of my talk, I will show on one emblematic example of a kagome antiferromagnet, herbertsmithite, $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$, how NMR can separate the contribution of defects from that of intrinsic properties and the unique outcomes which such experiments can bring.

Invited Talk AGjDPG 1.7 Tue 14:15 HSZ 04
Complex spin structures and multifunctional magnetism —
 ●VIVIEN ZAPF — National High Magnetic Field Lab, Los Alamos National Lab

There has been a recent surge of interest in multiferroics where magnetism and ferroelectricity are coupled to each other. In particular, complex magnetic spin textures such as skyrmions and other non-coplanar spin patterns can produce the necessary symmetry breaking to couple to ferroelectricity. I will discuss spatial inversion symmetry breaking in quantum and classical magnets and the microscopic coupling mechanisms between magnetism and ferroelectricity. I will review work at the National High Magnetic Field Lab, charting the phase diagrams of frustrated, quantum, and other complex spin systems to extended temperature and magnetic field which, conjunction with theory, can reveal important underlying information about the magnetic Hamiltonian.

AGjDPG 1.8 Tue 14:45 HSZ 04
Dimensional reduction due to geometric frustration – a case study — ●ULRICH TUTSCH¹, BURKHARD SCHMIDT², LARS POSTULKA¹, BERND WOLF¹, NATALIJA VAN WELL¹, FRANZ RITTER¹, CORNELIUS KRELLNER¹, WOLF ASSMUS¹, and MICHAEL LANG¹ — ¹Physikalisches Institut, Goethe-Universität Frankfurt, SFB/TR 49, 60438 Frankfurt (M), Germany — ²Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

Theoretical studies suggest that the frustrating zigzag bonds between the spin chains in triangular-lattice Heisenberg antiferromagnets gives rise to one-dimensional behaviour as long as $J'/J \leq 0.7$. $\text{Cs}_2\text{CuCl}_{4-x}\text{Br}_x$ ($0 \leq x \leq 4$) represents a good realization of such a system where the ratio J'/J of the in-plane spin-spin exchange coupling constants varies from 0.30 ($x = 0$) to 0.63 ($x = 2$), thus providing a well-suited model system for testing the frustration-induced dimensional-reduction scenario.

Here, we present specific heat data below 1 K for the compounds $\text{Cs}_2\text{CuCl}_2\text{Br}_2$ and $\text{Cs}_2\text{CuCl}_3\text{Br}$, which, due to site-selective substitution, show a well-ordered halide sublattice. The results for zero magnetic field for these systems as well as for the border compounds $x = 0$ and $x = 4$ can be well described by the antiferromagnetic Heisenberg chain model, fully consistent with frustration-induced one-dimensional behaviour.